LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049874.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.781	808	815	824	rVB	1035929	1652984	5.65%	0.463%
2	8.863	993	999	1004	rBV	340608	604702	2.07%	0.170%
3	8.957	1010	1015	1021	rBV	171744	327077	1.12%	0.092%
4	9.022	1021	1026	1034	rVB6	154642	368951	1.26%	0.103%
5	9.799	1152	1158	1166	rBV7	100951	295589	1.01%	0.083%
6	10.569	1282	1289	1299	rBV	1280714	2393028	8.18%	0.671%
7	10.898	1337	1345	1349	rBV3	108983	310988	1.06%	0.087%
8	10.963	1350	1356	1364	rVB3	188197	567881	1.94%	0.159%
9	11.146	1384	1387	1394	rVB3	173855	329232	1.13%	0.092%
10	11.498	1440	1447	1453	rBV4	284454	723416	2.47%	0.203%
11	11.575	1456	1460	1465	rVV3	170814	319549	1.09%	0.090%
12	11.734	1483	1487	1490	rBV2	220882	327429	1.12%	0.092%
13	11.822	1497	1502	1507	rBV	1280922	1905964	6.52%	0.534%
14	11.963	1520	1526	1529	rBV5	437863	941194	3.22%	0.264%
15	12.116	1549	1552	1556	rVB3	387736	536705	1.84%	0.150%
16	12.187	1559	1564	1566	rBV4	490066	875519	2.99%	0.245%
17	12.740	1655	1658	1664	rVB4	732724	1209292	4.14%	0.339%
18	12.792	1664	1667	1670	rBV2	305198	485389	1.66%	0.136%
19	12.851	1673	1677	1686	rBV2	1367505	3041786	10.40%	0.853%
20	12.957	1692	1695	1699	rVB2	534254	685301	2.34%	0.192%
21	13.334	1756	1759	1763	rVB	608474	659855	2.26%	0.185%
22	13.387	1764	1768	1772	rBV	667987	951383	3.25%	0.267%
23	13.469	1777	1782	1783	rBV2	1407009	2073850	7.09%	0.581%
24	13.581	1797	1801	1805	rBV4	618234	947929	3.24%	0.266%
25	13.898	1851	1855	1859	rBV4	716423	995309	3.40%	0.279%
26	14.198	1903	1906	1910	rBV2	565478	727668	2.49%	0.204%
27	14.381	1935	1937	1940	rBV	366044	423513	1.45%	0.119%
28	14.422	1940	1944	1948	rVB	2071023	2823514	9.66%	0.792%
29	14.604	1972	1975	1979	rVB	697870	798702	2.73%	0.224%
30	15.369	2102	2105	2111	rVB2	1353102	2324748	7.95%	0.652%
31	15.845	2183	2186	2191	rBV2	1257700	1904822	6.51%	0.534%
32	16.057	2219	2222	2226	rVB	2559365	2770380	9.47%	0.777%
33	16.263	2253	2257	2262	rVB3	1483753	2657216	9.09%	0.745%
34	16.333	2265	2269	2277	rVB	3251094	5352657	18.30%	1.501%
35	16.410	2279	2282	2286	rBV2	1833422	2656597	9.08%	0.745%
36	16.569	2305	2309	2317	rVB2	2677282	4707986	16.10%	1.320%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.763	2339	2342	2346	rBV	1561481	2034004	6.96%	0.570%
38	16.828	2350	2353	2359	rVB3	1207182	2035123	6.96%	0.571%
39	16.928	2367	2370	2377	rVB	1641993	2811778	9.61%	0.788%
40	17.075	2391	2395	2402	rBV2	6084879	9989483	34.16%	2.800%
41	17.180	2408	2413	2419	rBV3	5555372	12142221	41.52%	3.404%
42	17.239	2420	2423	2432	rVB4	3906710	8647854	29.57%	2.424%
43	17.339	2433	2440	2443	rBV3	4558476	7840884	26.81%	2.198%
44	17.375	2444	2446	2448	rBV	1581430	1694487	5.79%	0.475%
45	17.445	2455	2458	2461	rBV	1773237	2059203	7.04%	0.577%
46	17.486	2461	2465	2470	rBV3	2893499	5740720	19.63%	1.609%
47	17.545	2471	2475	2482	rBV3	6378601	14522969	49.66%	4.071%
48	17.710	2496	2503	2509	rBV	6427380	15060790	51.50%	4.222%
49	17.839	2520	2525	2531	rBV2	16436807	29244024	100.00%	8.198%
50	17.951	2541	2544	2545	rBV	2301633	2576069	8.81%	0.722%
51	18.269	2595	2598	2601	rVB	3561247	3756904	12.85%	1.053%
52	18.551	2642	2646	2649	rBV	9188510	11614815	39.72%	3.256%
53	19.227	2759	2761	2765	rVB2	3752272	4142820	14.17%	1.161%
54	19.310	2773	2775	2779	rVB2	2977226	2932215	10.03%	0.822%
55	19.539	2811	2814	2817	rBV3	3338045	4548104	15.55%	1.275%
56	20.486	2973	2975	2978	rBV3	3117286	3881007	13.27%	1.088%
57	20.857	3035	3038	3042	rVB2	4021937	5458591	18.67%	1.530%
58	21.127	3081	3084	3093	rVB6	5337578	11303597	38.65%	3.169%
59	21.198	3093	3096	3098	rBV2	4683764	5676072	19.41%	1.591%
60	21.421	3130	3134	3138	rVB4	9556900	17315745	59.21%	4.854%
61	21.633	3166	3170	3179	rVB4	8238029	17724215	60.61%	4.969%
62	21.727	3181	3186	3191	rBV3	8000012	15944347	54.52%	4.470%
63	21.951	3220	3224	3232	rVB2	7808847	14862237	50.82%	4.166%
64	22.051	3236	3241	3251	rVB6	6602911	18618820	63.67%	5.219%
65	22.298	3278	3283	3289	rBV4	8322180	16010289	54.75%	4.488%
66	22.674	3342	3347	3355	rVB2	6559579	14125747	48.30%	3.960%
67	22.945	3388	3393	3405	rVB4	5860549	13412840	45.87%	3.760%
68	23.380	3462	3467	3474	rVB2	4090981	8312323	28.42%	2.330%

Sum of corrected areas: 356718402

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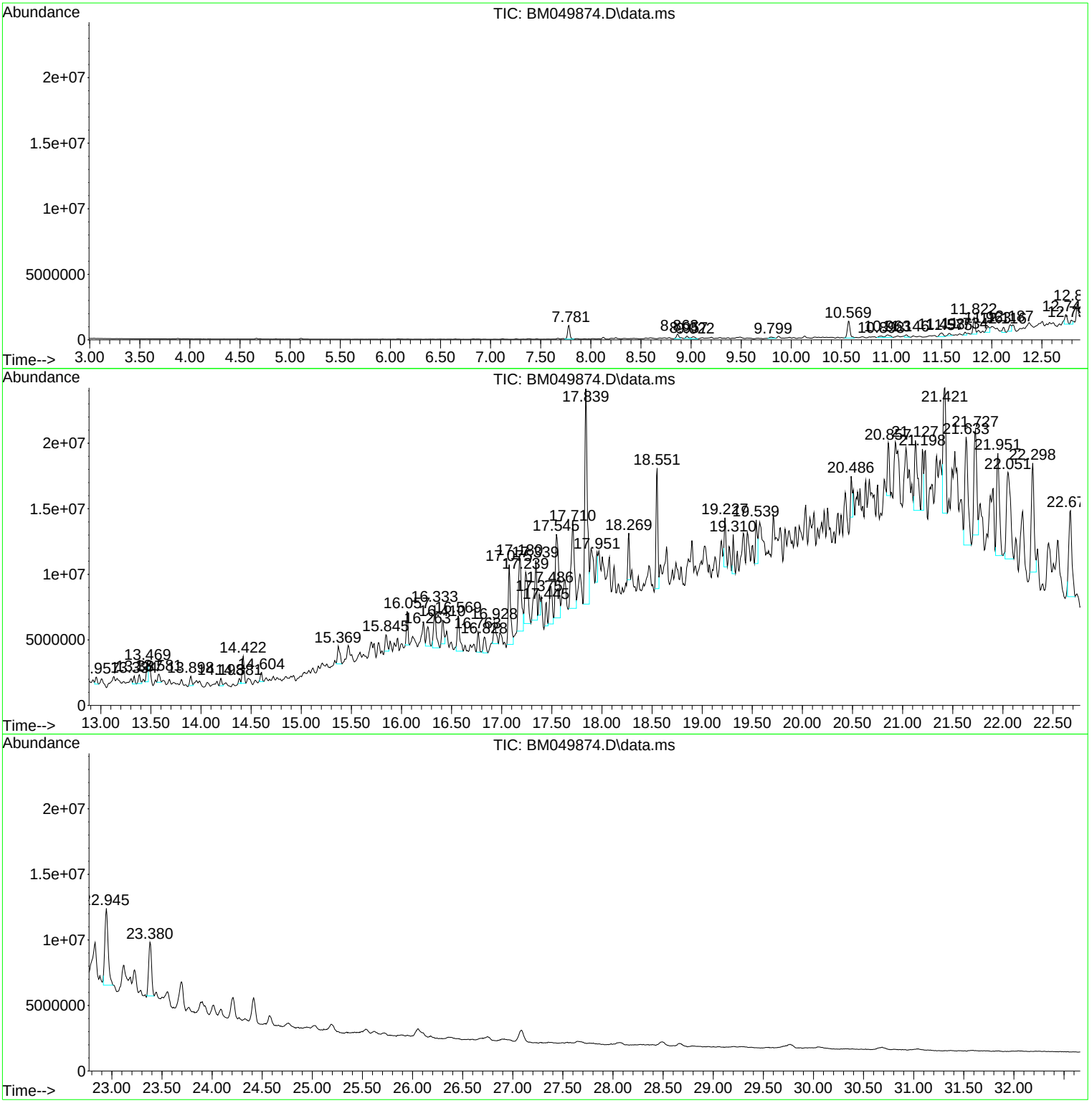
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
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Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

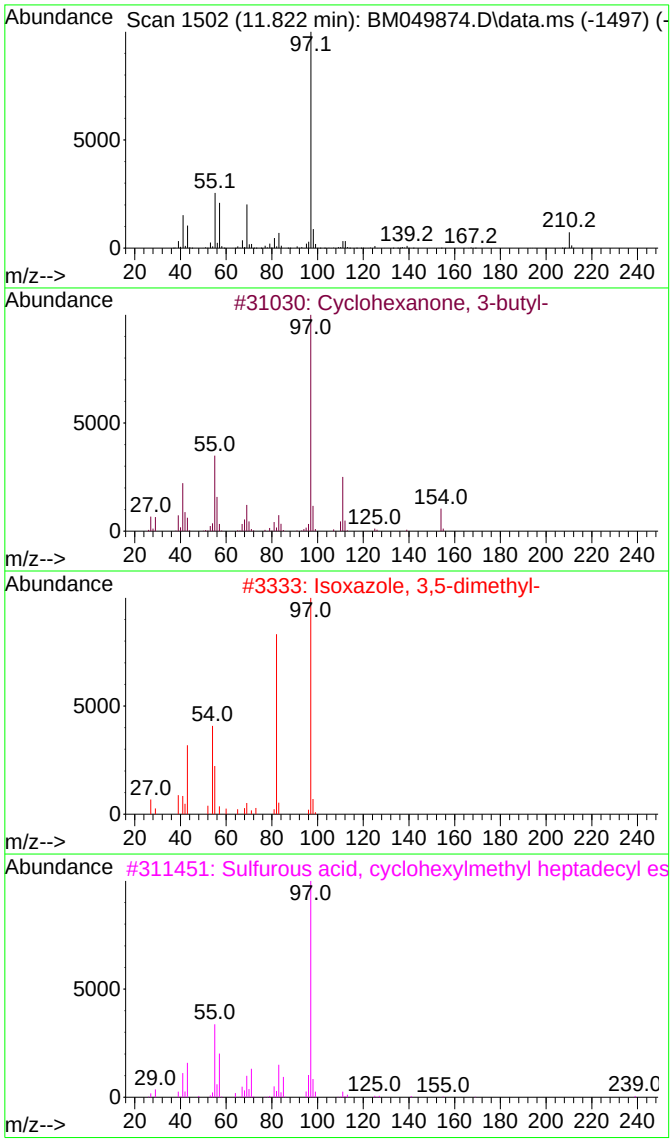
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

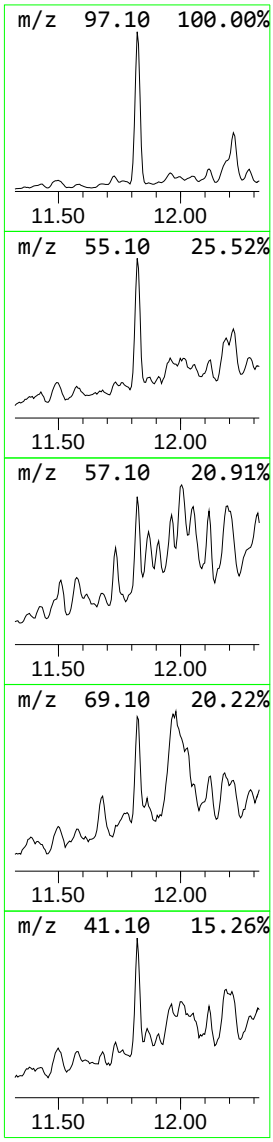
****

Peak Number 1 Cyclohexanone, 3-butyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	15.93 ng	1905960	Naphthalene-d8	10.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	72
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	64
3	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	56
4	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	56
5	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

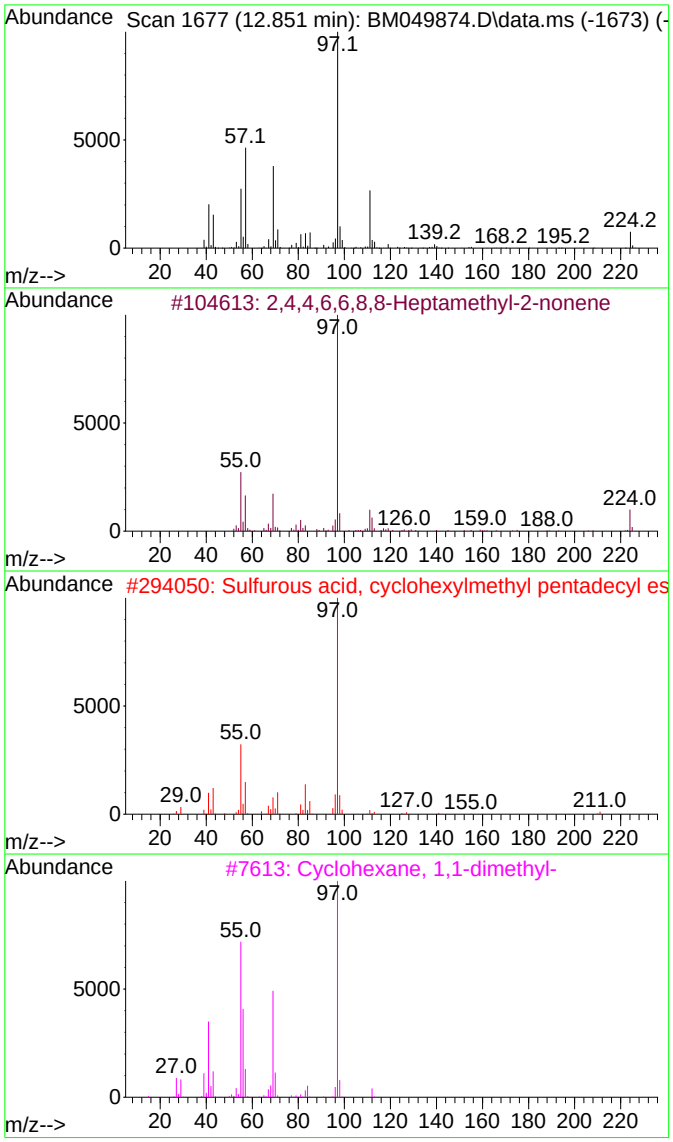
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

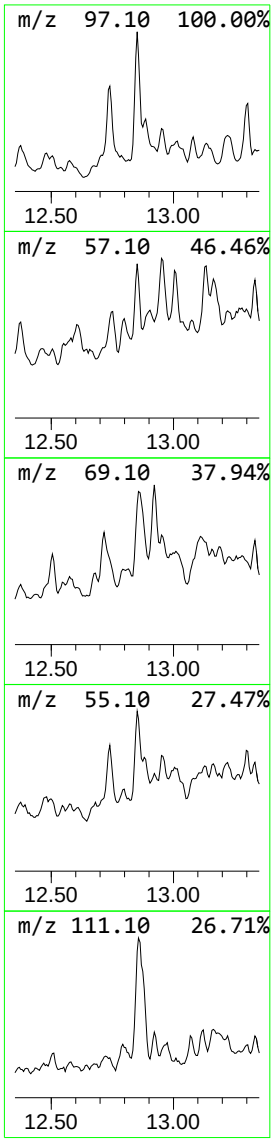
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-2... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.851	21.55 ng	3041790	Acenaphthene-d10	14.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	74
2	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	59
3	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	53
4	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	53
5	1,1-Dimethyl-1-silacyclo-3-pentene	112	C6H12Si	016054-12-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

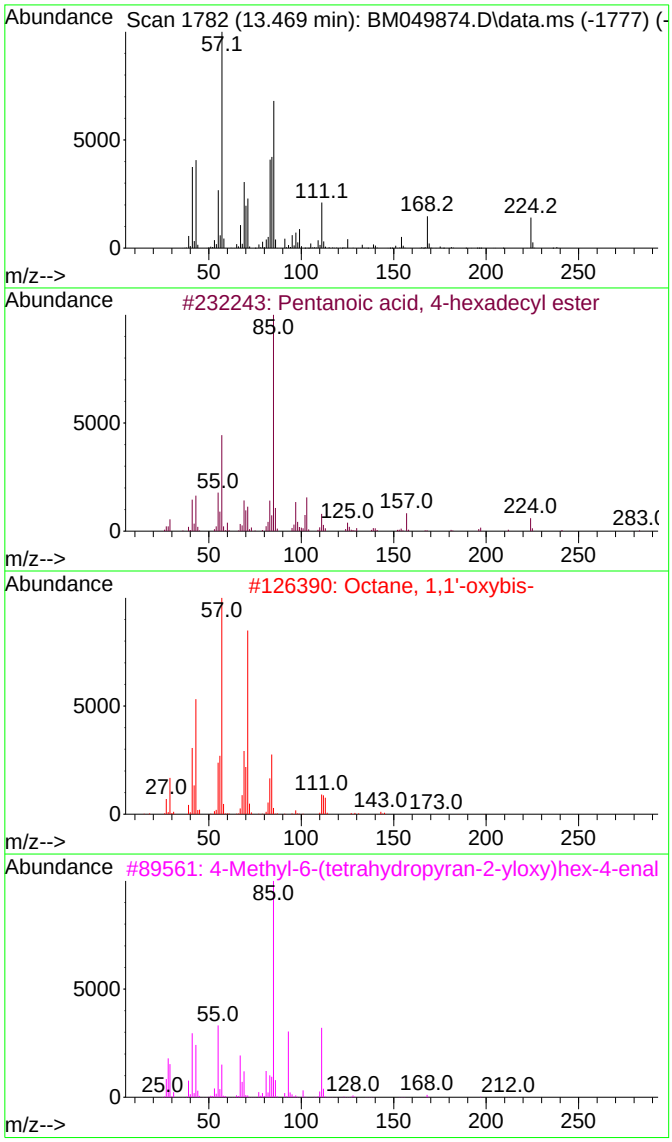
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

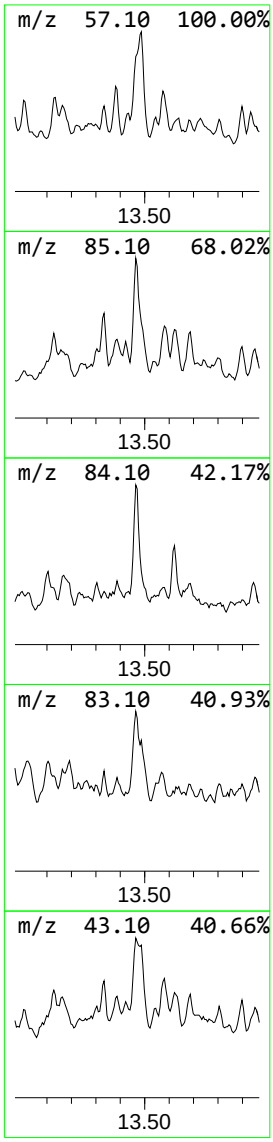
****

Peak Number 3 unknown13.469 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.469	14.69 ng	2073850	Acenaphthene-d10	14.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4-hexadecyl ester	326	C21H42O2	1000282-86-4	40
2	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	27
3	4-Methyl-6-(tetrahydropyran-2-yl...	212	C12H20O3	064218-01-5	27
4	2-Butene, 1,4-diethoxy-	144	C8H16O2	007250-85-3	25
5	2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

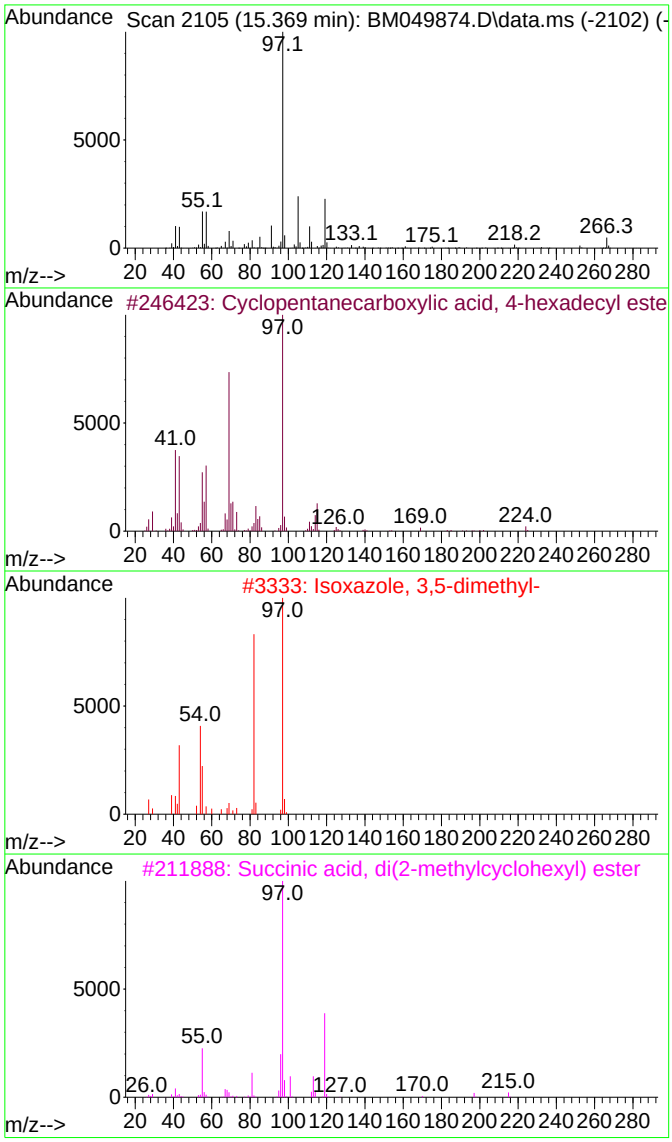
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

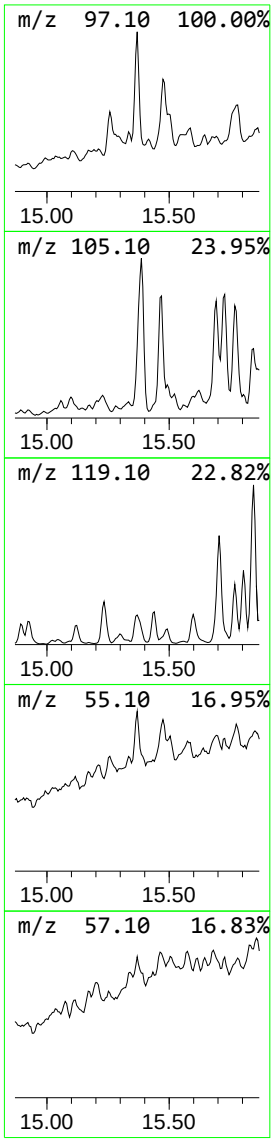
****

Peak Number 4 unknown15.369 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.369	16.47 ng	2324750	Acenaphthene-d10	14.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	43
2	Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	38
3	Succinic acid, di(2-methylcycloh...	310	C18H30O4	1000329-83-0	38
4	2,4,4,6,6,8,8-Heptamethyl-2-nonene	224	C16H32	039761-73-4	38
5	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

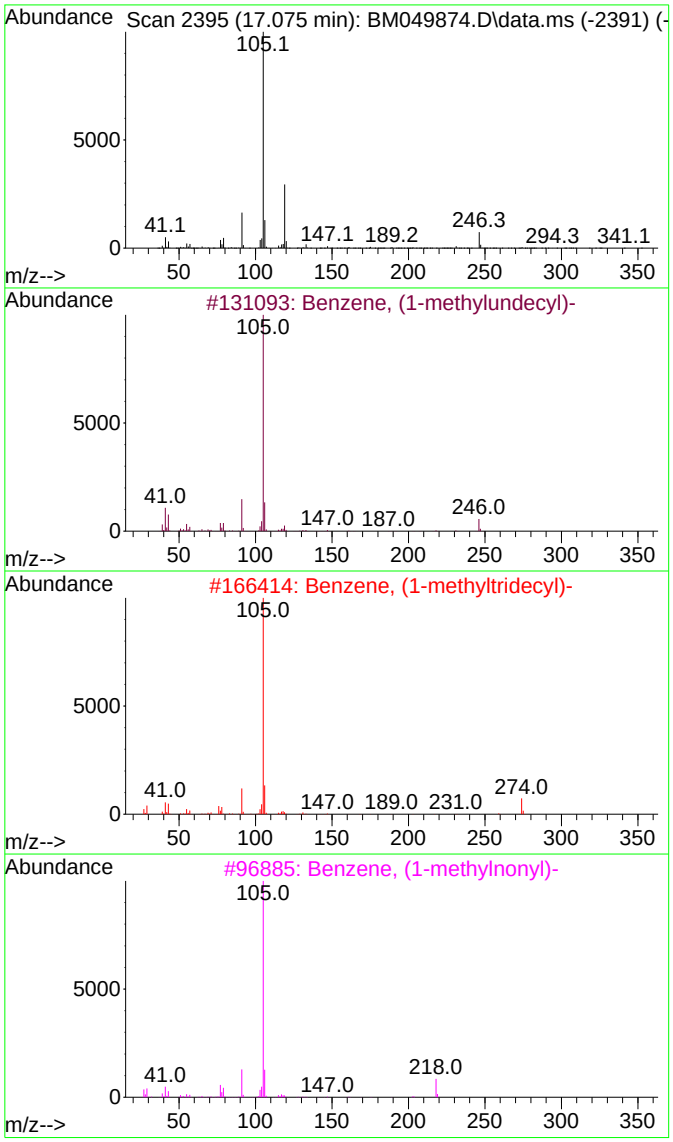
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

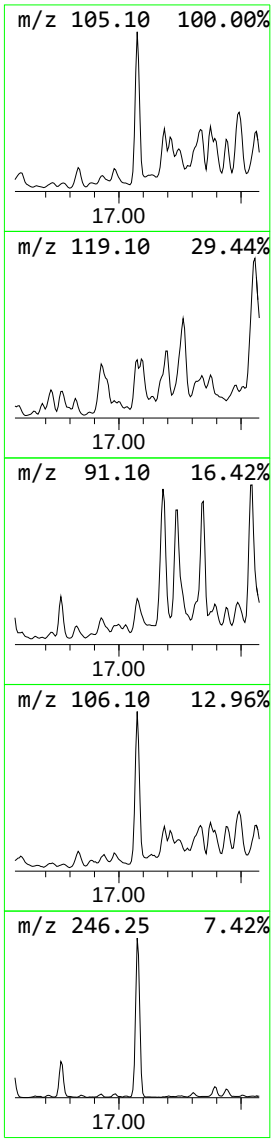
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (1-methylundecyl)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.075	16.45 ng	9989480	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	70
2	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	53
3	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	47
4	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	47
5	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

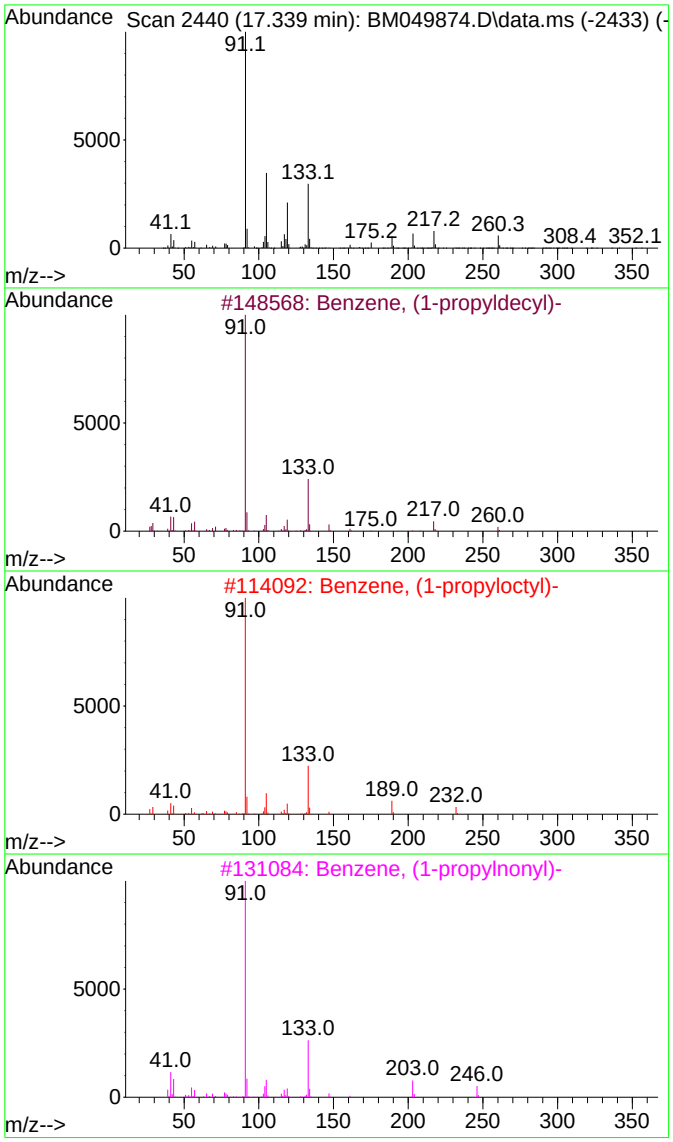
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

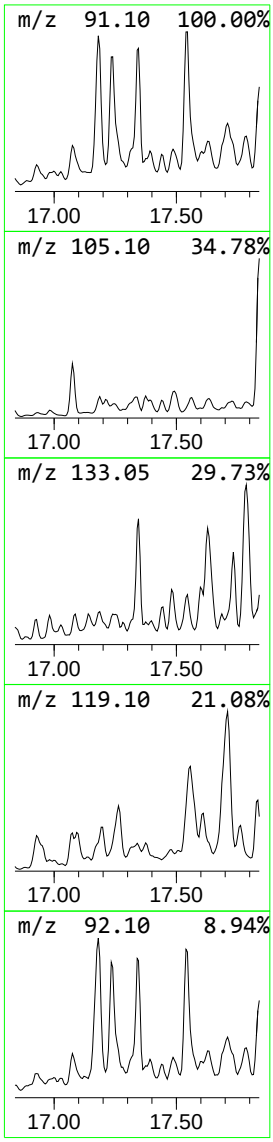
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (1-propyldecyl)- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.339	12.92 ng	7840880	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-propyldecyl)-	260	C19H32	004534-51-4	53
2	Benzene, (1-propyloctyl)-	232	C17H28	004536-86-1	43
3	Benzene, (1-propylnonyl)-	246	C18H30	002719-64-4	43
4	Benzene, (1-hexylheptyl)-	260	C19H32	002400-01-3	38
5	Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

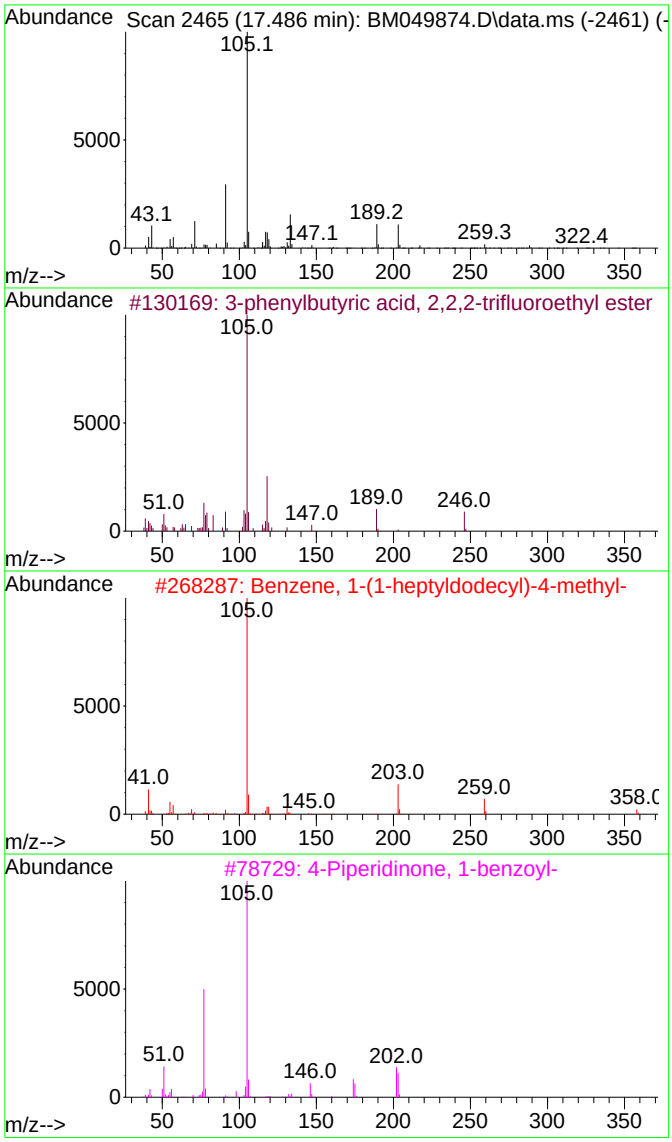
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

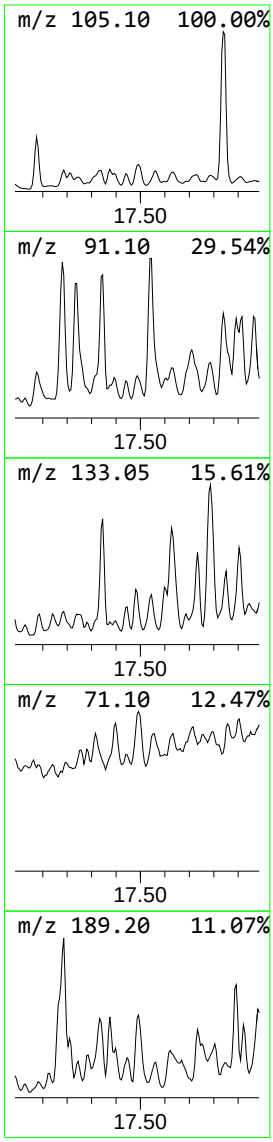
****

Peak Number 7 unknown17.486 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.486	9.46 ng	5740720	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-phenylbutyric acid, 2,2,2-trif...	246	C12H13F3O2	1000376-55-4	43
2	Benzene, 1-(1-heptyldodecyl)-4-m...	358	C26H46	055191-36-1	37
3	4-Piperidinone, 1-benzoyl-	203	C12H13NO2	024686-78-0	27
4	4,5-Dihydro-4,4-dimethyl-2-pheny...	203	C12H13NO2	029637-55-6	25
5	3-Phenylpropionic acid, 2,3,4,6-...	362	C15H10Cl4O2	1000354-74-6	16





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Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

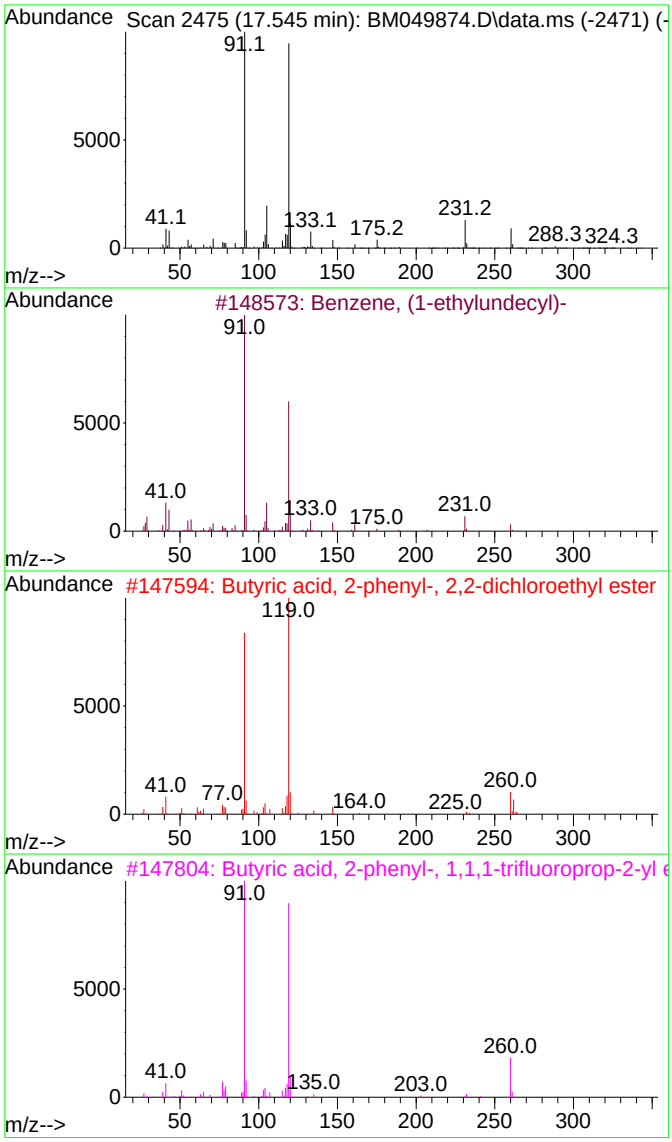
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

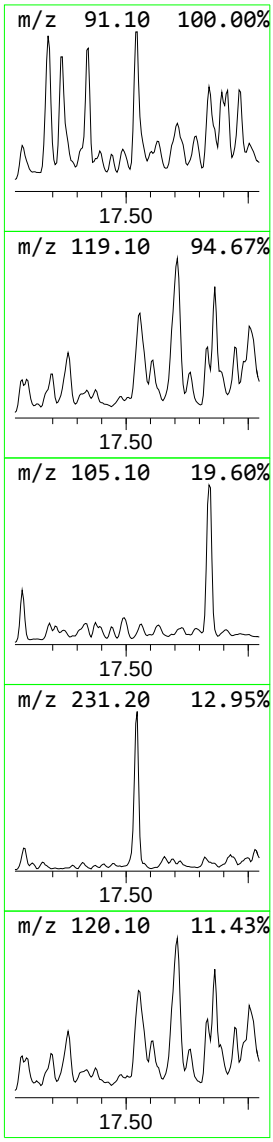
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, (1-ethylundecyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.545	23.92 ng	14523000	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	94
2	Butyric acid, 2-phenyl-, 2,2-dic...	260	C12H14Cl2O2	1000406-85-7	76
3	Butyric acid, 2-phenyl-, 1,1,1-t...	260	C13H15F3O2	1000406-85-1	76
4	Benzamide, 2-methyl-N-allyl-N-bu...	231	C15H21NO	1010446-30-9	59
5	Butyric acid, 2-phenyl-, 2-methy...	286	C19H26O2	1000406-91-8	53





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Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

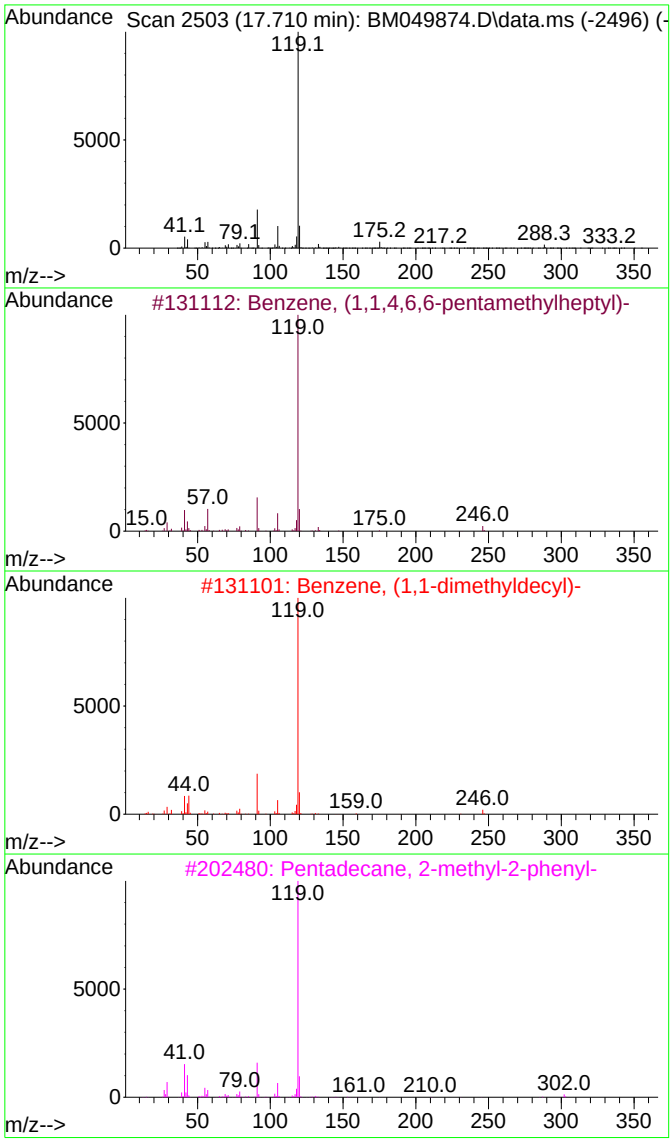
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

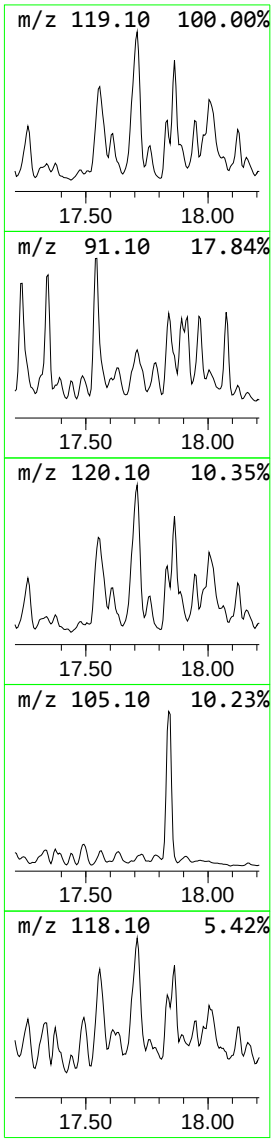
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1,1,4,6,6-pentame... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.710	24.81 ng	15060800	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1,1,4,6,6-pentamethylh...	246	C18H30	055134-07-1	91
2	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	87
3	Pentadecane, 2-methyl-2-phenyl-	302	C22H38	029138-94-1	78
4	Dicumyl peroxide	270	C18H22O2	000080-43-3	72
5	3-Methylbenzoic acid, 2,5-dichlo...	280	C14H10Cl2O2	1000325-71-3	72





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Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

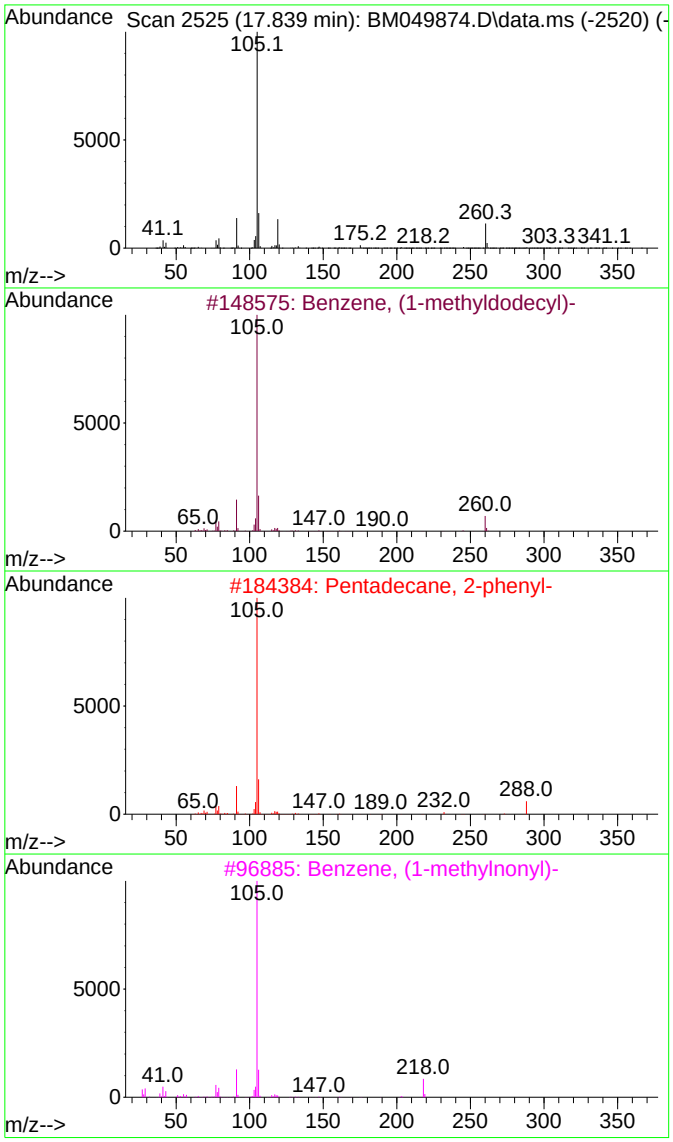
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

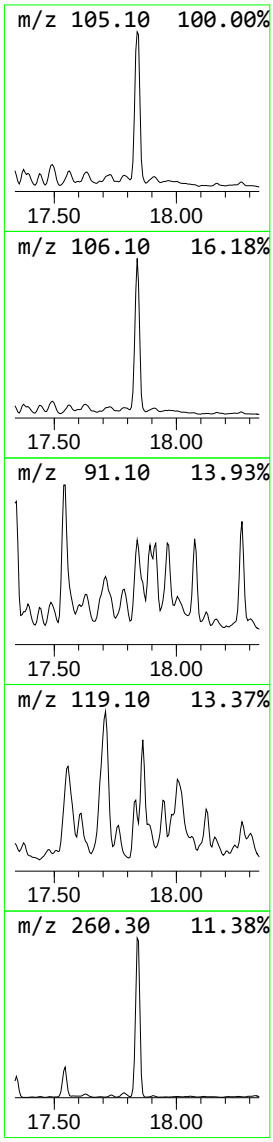
****

Peak Number 10 Benzene, (1-methyldodecyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.839	48.17 ng	29244000	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	81
2	Pentadecane, 2-phenyl-	288	C21H36	004534-66-1	62
3	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	50
4	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	50
5	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	50





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Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

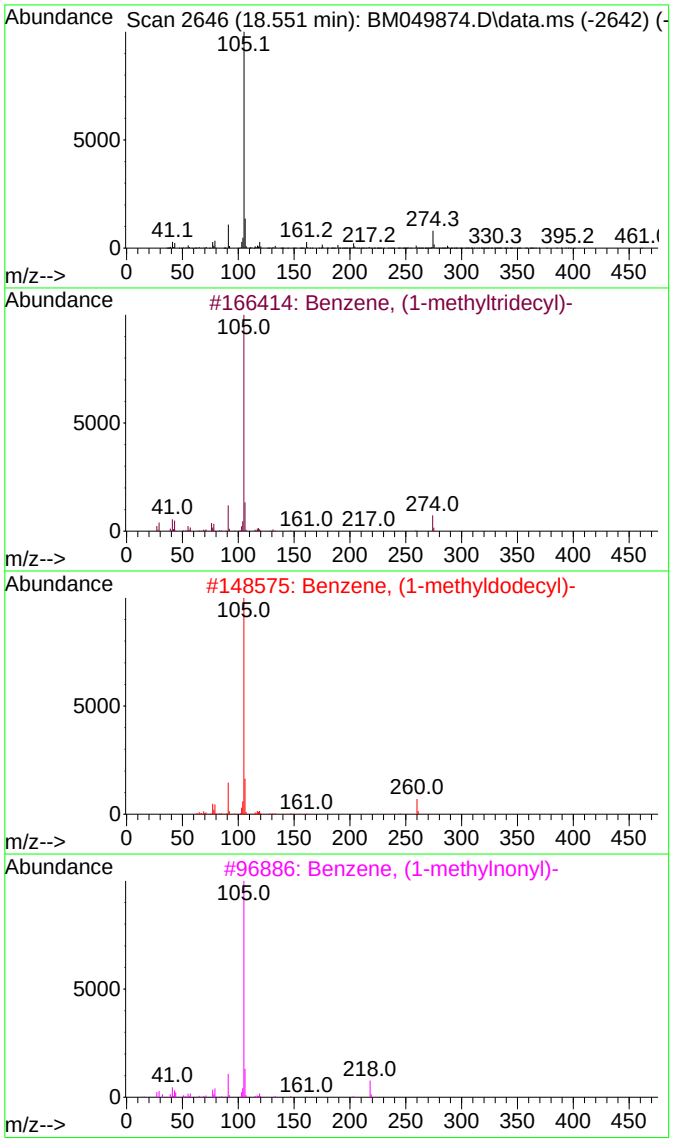
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

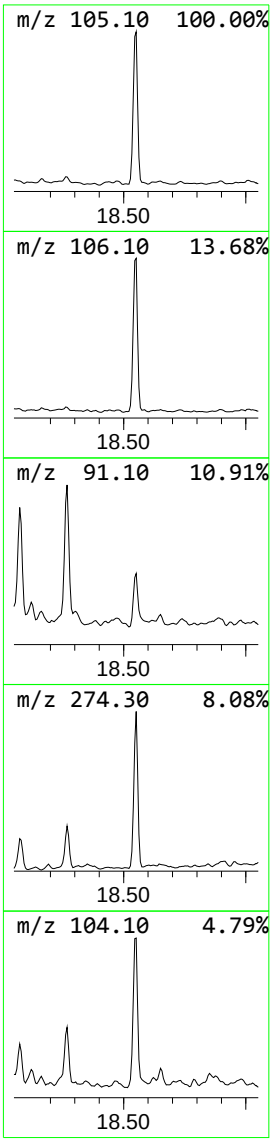
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, (1-methyltridecyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.551	19.13 ng	11614800	Phenanthrene-d10	17.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyltridecyl)-	274	C20H34	004534-59-2	74
2	Benzene, (1-methyldodecyl)-	260	C19H32	004534-53-6	70
3	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	53
4	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	53
5	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	53





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Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

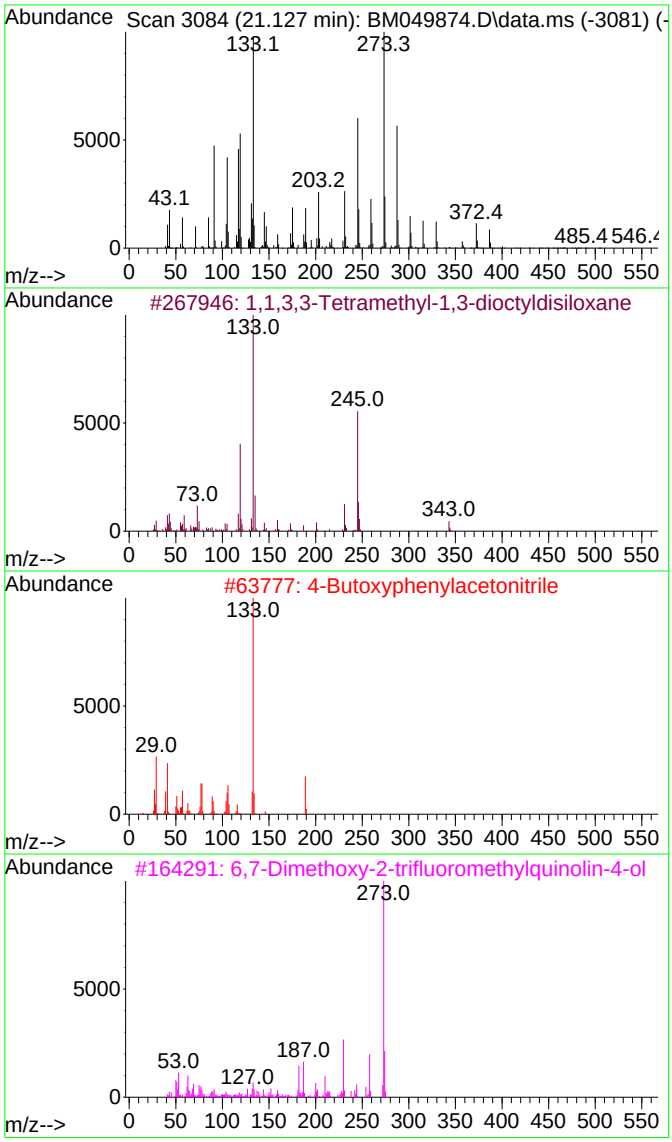
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

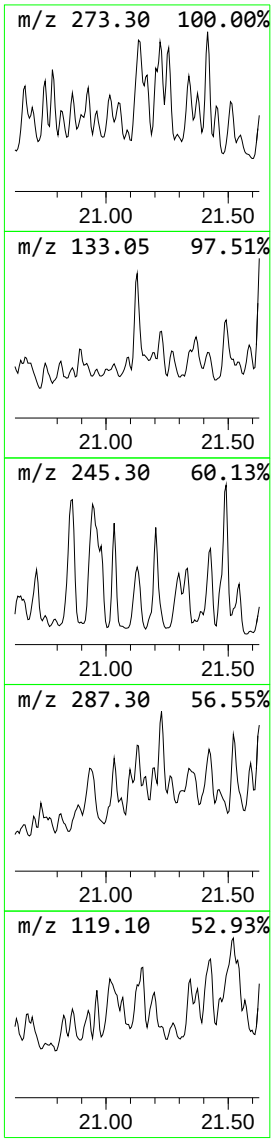
****

Peak Number 12 unknown21.127 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	13.06 ng	11303600	Chrysene-d12	21.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,3,3-Tetramethyl-1,3-dioctyld...	358	C20H46OSi2	018642-94-9	27
2	4-Butoxyphenylacetonitrile	189	C12H15NO	038746-93-9	11
3	6,7-Dimethoxy-2-trifluoromethylq...	273	C12H10F3NO3	041192-83-0	11
4	3,4-Diaminobenzonitrile	133	C7H7N3	017626-40-3	11
5	1,2,4-Oxadiazol-5(4H)-one, 4-(2-...	273	C13H8ClN3O2	288246-55-9	11





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Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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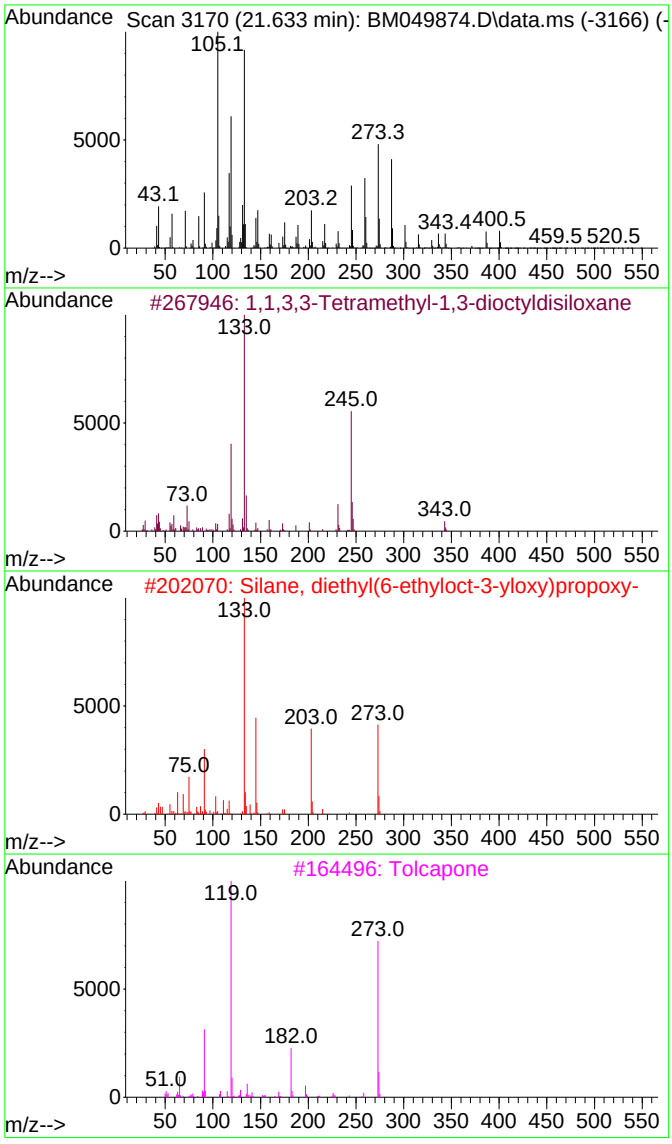
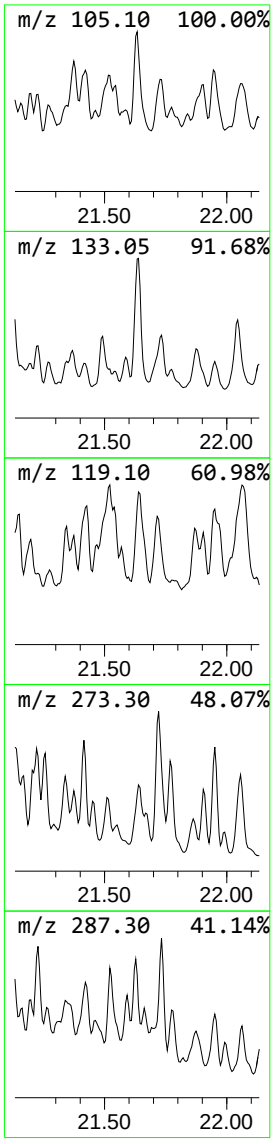
Peak Number 13 unknown21.633 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.633	20.47 ng	17724200	Chrysene-d12	21.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,3,3-Tetramethyl-1,3-dioctyld...	358	C20H46OSi2	018642-94-9	38
2	Silane, diethyl(6-ethyloct-3-ylo...	302	C17H38O2Si	1000363-01-5	35
3	Tolcapone	273	C14H11NO5	134308-13-7	18
4	Ethanone, 1-phenyl-2-phenylsulfo...	274	C14H14N2O2S	1000269-86-8	18
5	Benzamide, 4-ethyl-N-(2-butyl)-N...	289	C19H31NO	1000464-16-5	14





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Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

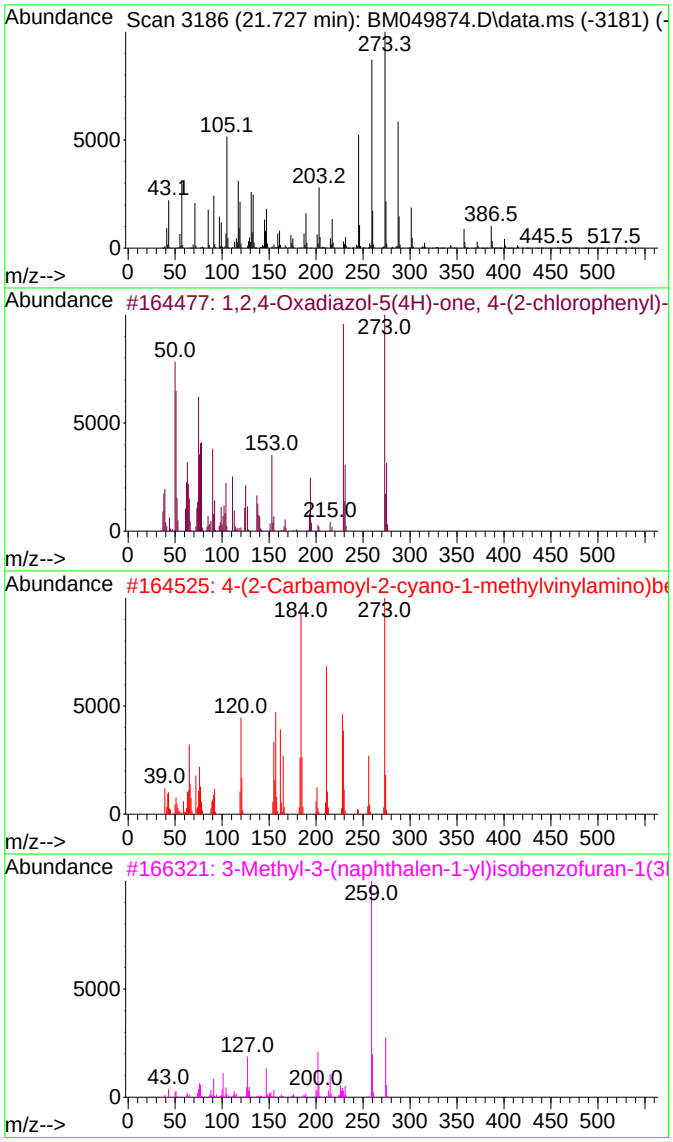
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

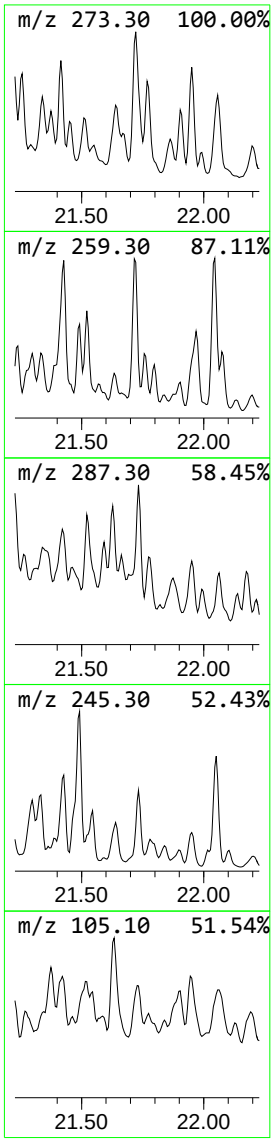
****

Peak Number 14 unknown21.727 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.727	18.42 ng	15944300	Chrysene-d12	21.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Oxadiazol-5(4H)-one, 4-(2-...	273	C13H8ClN3O2	288246-55-9	35
2	4-(2-Carbamoyl-2-cyano-1-methylv...	273	C14H15N3O3	1000311-98-1	35
3	3-Methyl-3-(naphthalen-1-yl)isob...	274	C19H14O2	078772-71-1	30
4	Bi-1-cyclohexen-1-yl, 3,3,3',3',...	274	C20H34	076993-52-7	30
5	Propanamide, N-(1-ethyl-1,2,3,4-...	274	C17H26N2O	063134-09-8	25





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Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

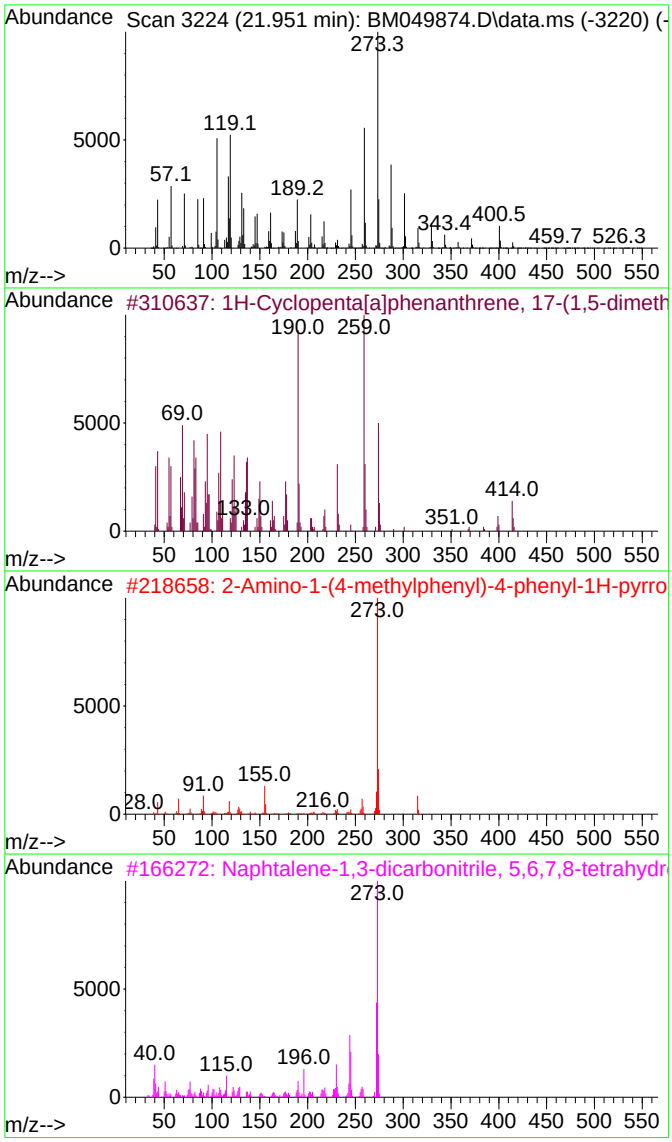
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

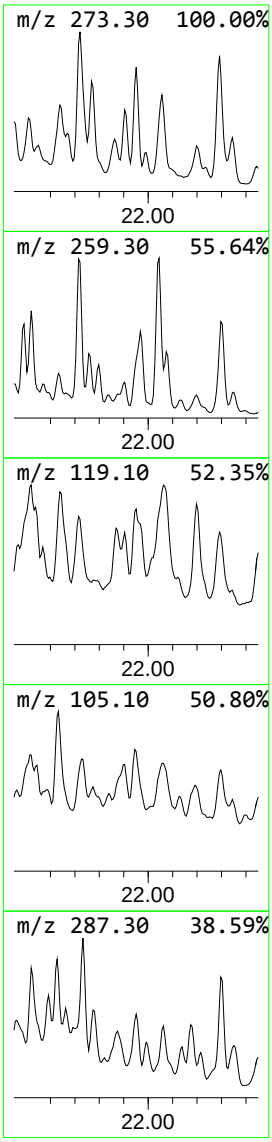
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 1H-Cyclopenta[a]phenanthren... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.951	17.17 ng	14862200	Chrysene-d12	21.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopenta[a]phenanthrene, 17...	414	C30H54	000474-20-4	91
2	2-Amino-1-(4-methylphenyl)-4-phe...	315	C20H17N3O	1000479-67-7	38
3	Naphtalene-1,3-dicarbonitrile, 5...	274	C18H14N2O	1000259-78-7	30
4	Euparin, TMS derivative	288	C16H20O3Si	1000478-60-9	30
5	Silane, diethylheptyloxy(2-hexyl...	302	C17H38O2Si	1000363-50-2	27





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Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

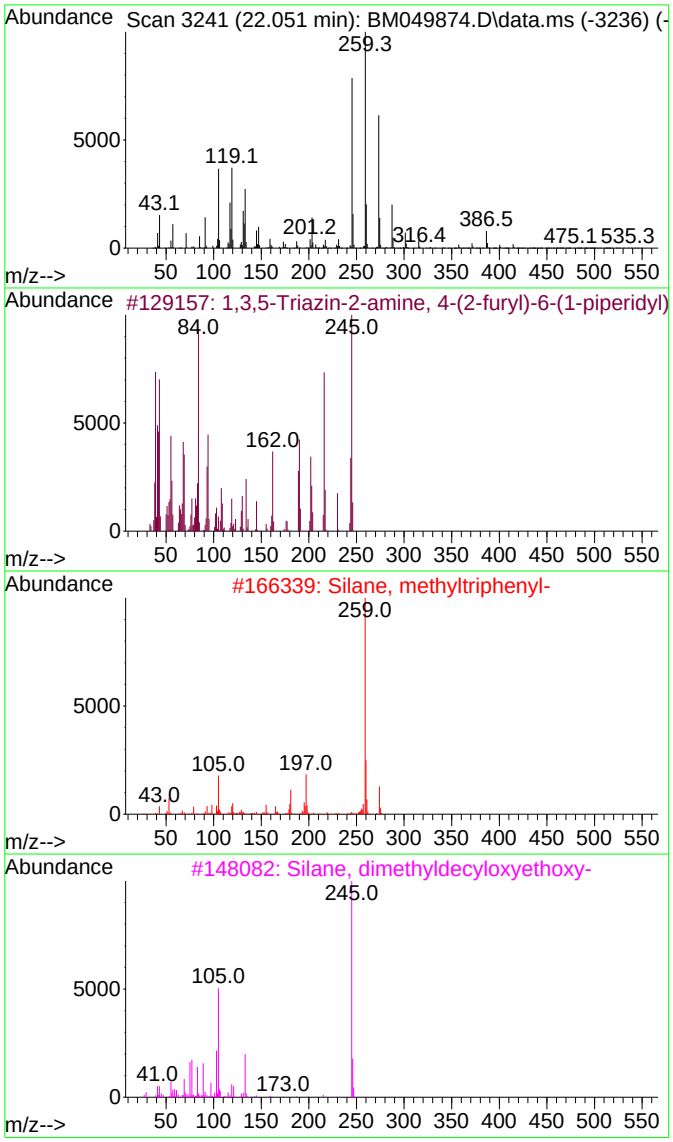
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

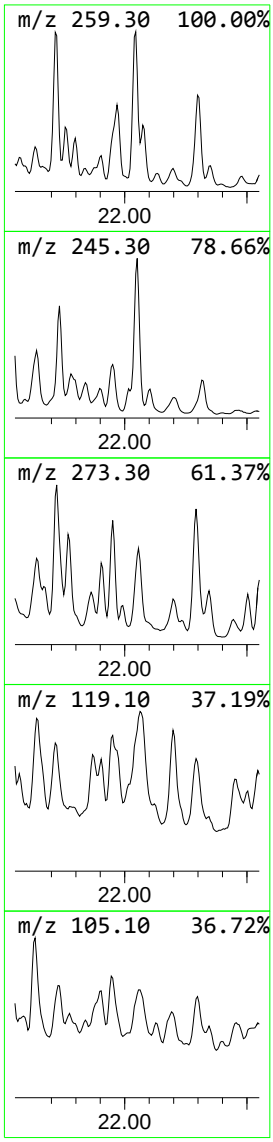
****

Peak Number 16 unknown22.051 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.051	21.51 ng	18618800	Chrysene-d12	21.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazin-2-amine, 4-(2-fury...	245	C12H15N5O	148403-53-6	25
2	Silane, methyltriphenyl-	274	C19H18Si	000791-29-7	22
3	Silane, dimethyldecyloxyethoxy-	260	C14H32O2Si	1000346-91-9	22
4	1,4-Benzenediamine, N,N-dimethyl...	259	C13H13N3O3	126893-37-6	18
5	Pyrimidine-2,4,6(1H,3H,5H)-trion...	274	C13H14N4O3	346612-04-2	18





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Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

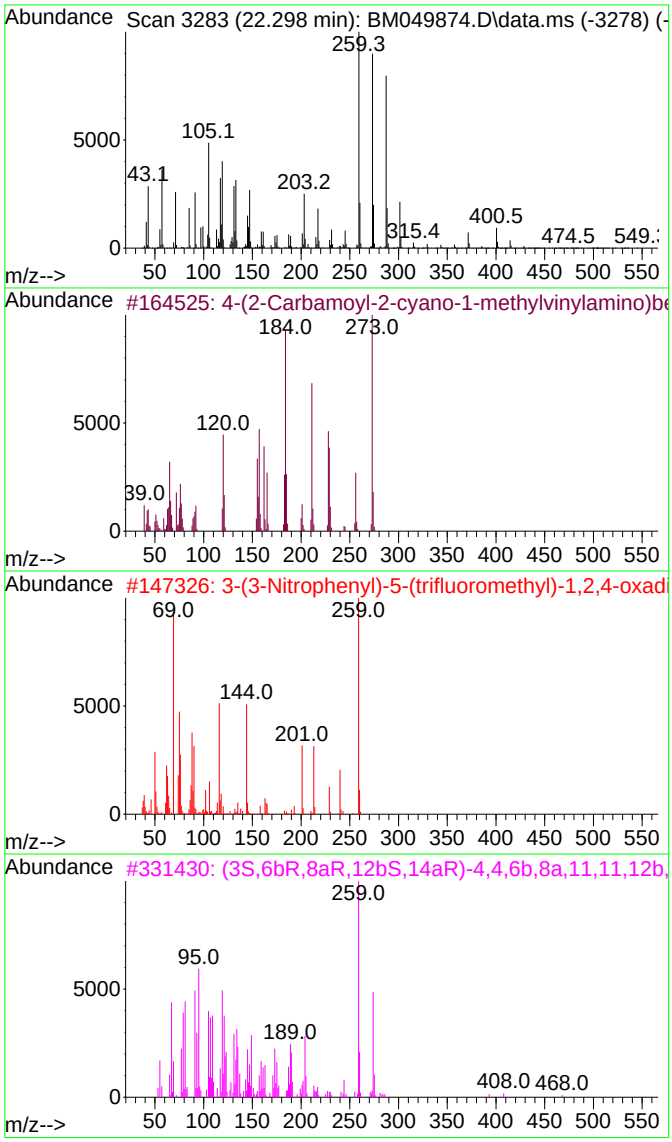
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

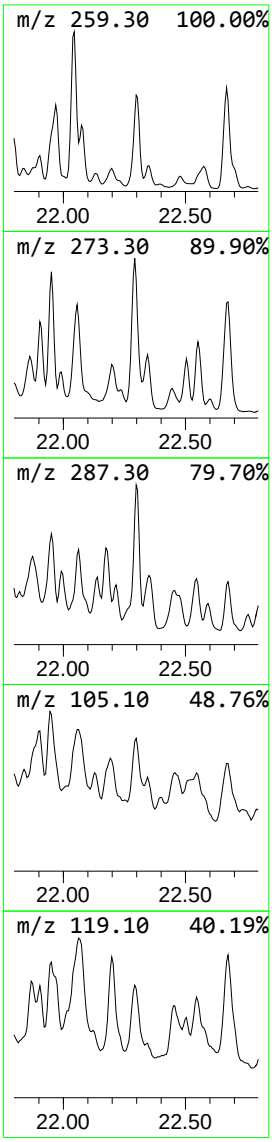
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 4-(2-Carbamoyl-2-cyano-1-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.298	18.49 ng	16010300	Chrysene-d12	21.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(2-Carbamoyl-2-cyano-1-methylv...	273	C14H15N3O3	1000311-98-1	53
2	3-(3-Nitrophenyl)-5-(trifluorome...	259	C9H4F3N3O3	071754-22-8	25
3	(3S,6bR,8aR,12bS,14aR)-4,4,6b,8a...	468	C32H52O2	1000441-99-4	18
4	3-Methyl-3-(naphthalen-1-yl)isob...	274	C19H14O2	078772-71-1	18
5	Propanamide, N-(1-ethyl-1,2,3,4-...	274	C17H26N2O	063134-09-8	18





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Operator : RC/JU
Sample : Q1739-01 20X
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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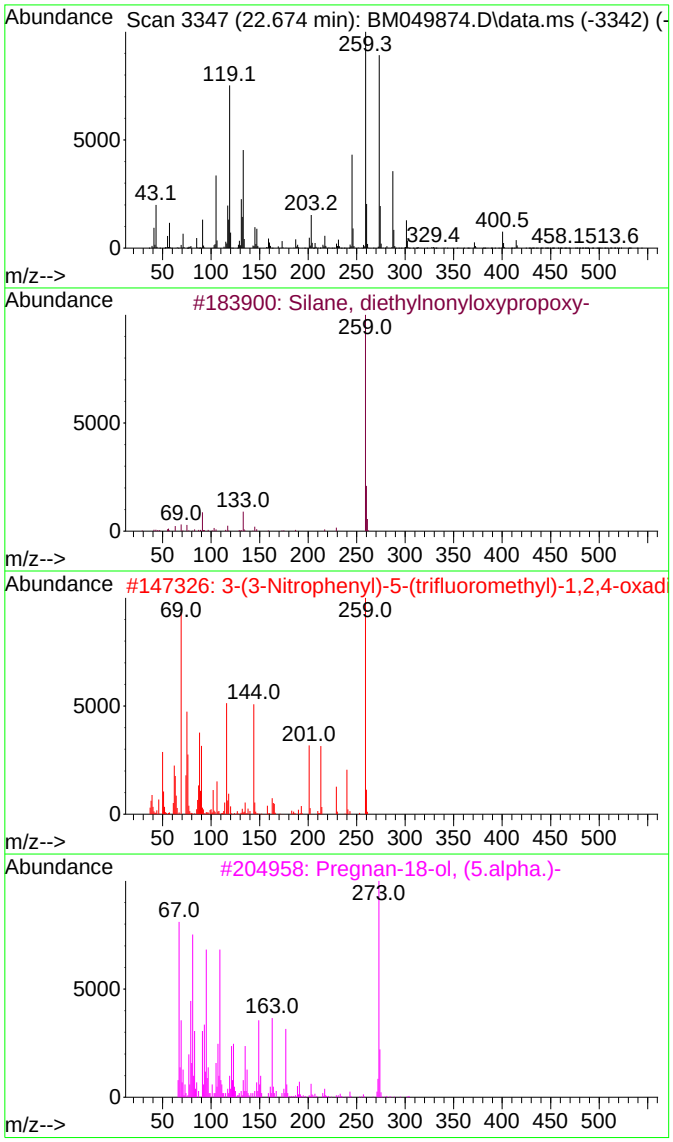
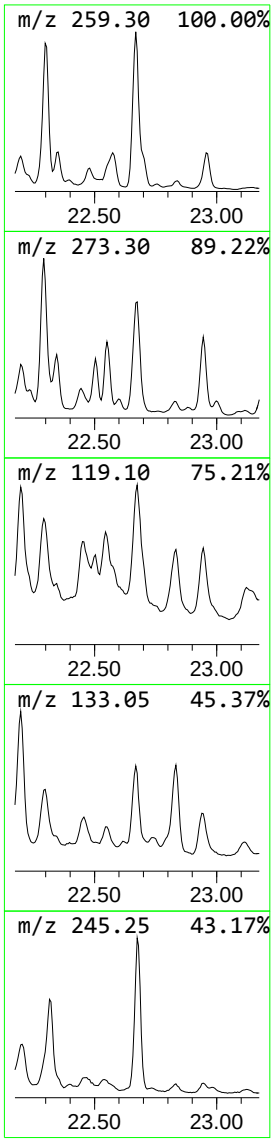
Peak Number 18 unknown22.674 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.674	16.32 ng	14125700	Chrysene-d12	21.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, diethylnonyloxypropoxy-	288	C16H36O2Si	1010363-08-5	22
2	3-(3-Nitrophenyl)-5-(trifluorome...	259	C9H4F3N3O3	071754-22-8	11
3	Pregnan-18-ol, (5.alpha.)-	304	C21H36O	056053-09-9	11
4	3Ah-pyrrolo[3,4-d]isoxazole-3-ca...	274	C13H10N2O5	1010317-17-8	11
5	Diglycolic acid, 2-acetylphenyl ...	406	C23H34O6	1000382-72-7	11





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Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

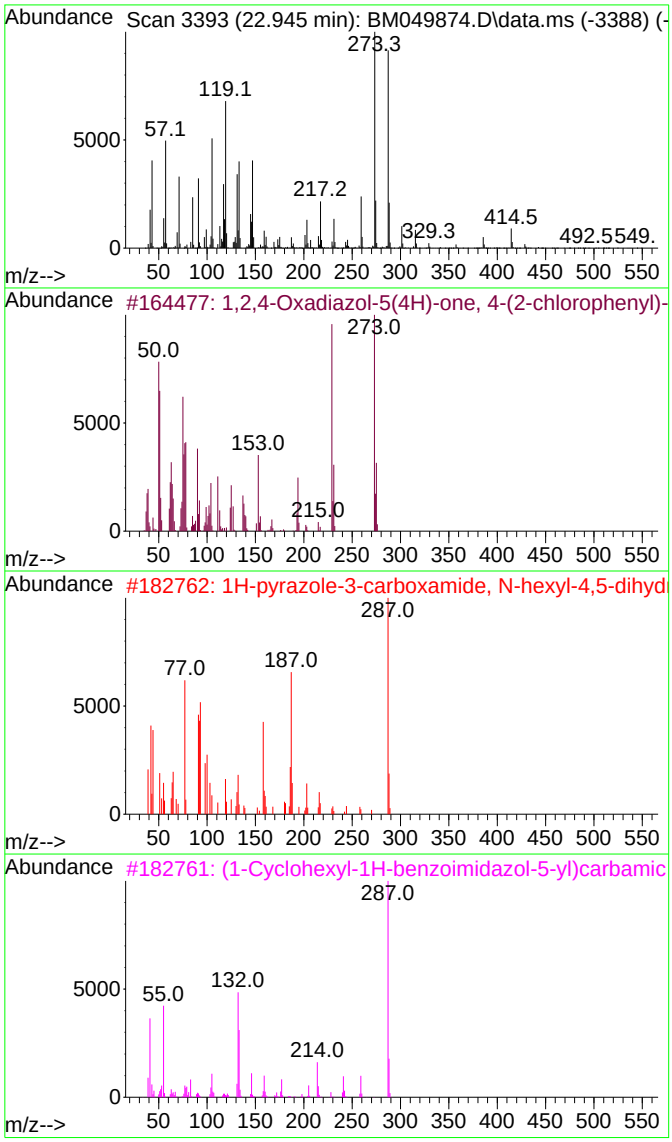
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

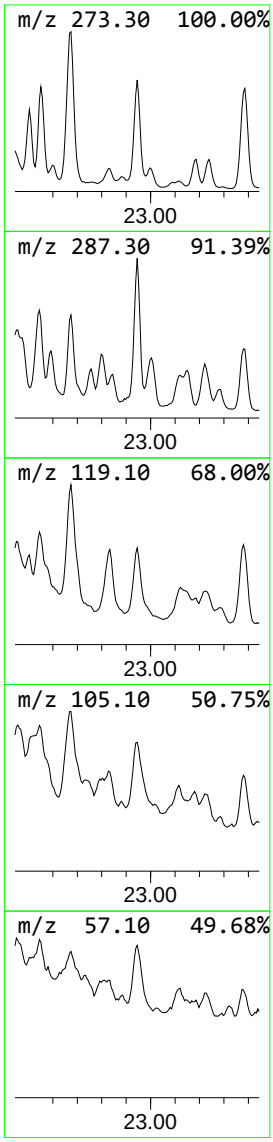
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 1,2,4-Oxadiazol-5(4H)-one, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.945	32.27 ng	13412800	Perylene-d12	24.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Oxadiazol-5(4H)-one, 4-(2-...	273	C13H8ClN3O2	288246-55-9	56
2	1H-pyrazole-3-carboxamide, N-hex...	287	C16H21N3O2	1000397-27-6	25
3	(1-Cyclohexyl-1H-benzoimidazol-5...	287	C16H21N3O2	1000310-00-5	25
4	4-Amino-3-ethyl-1,2,4-triazole-5...	288	C10H24N4SSi2	1000479-88-4	22
5	Pyridinitril	273	C13H5Cl2N3	001086-02-8	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

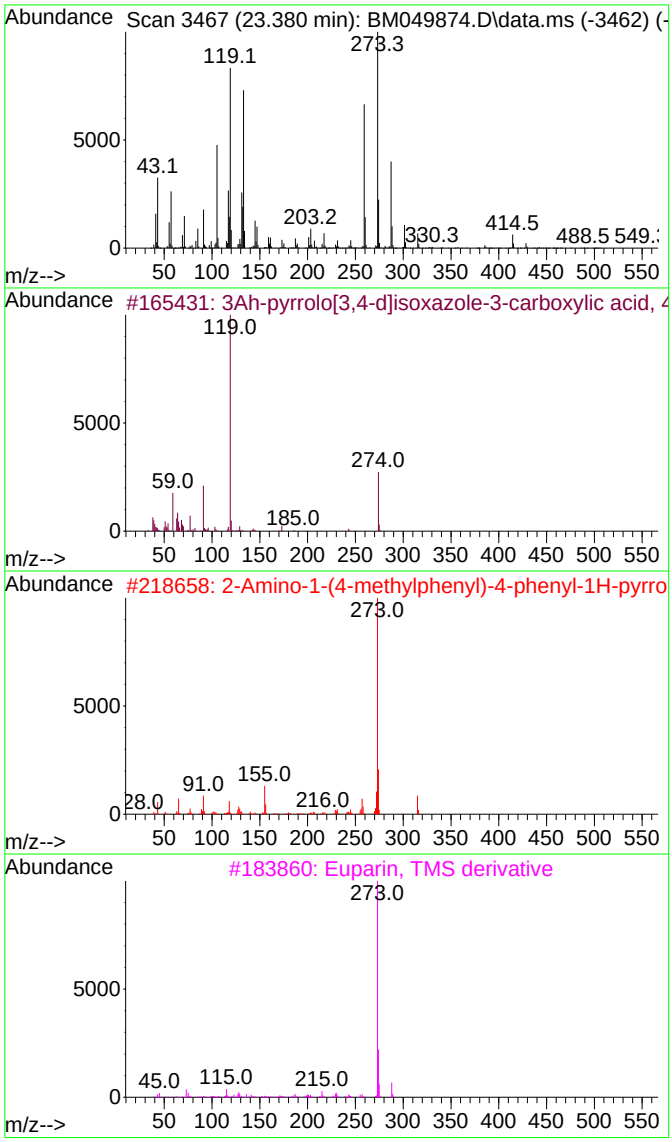
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

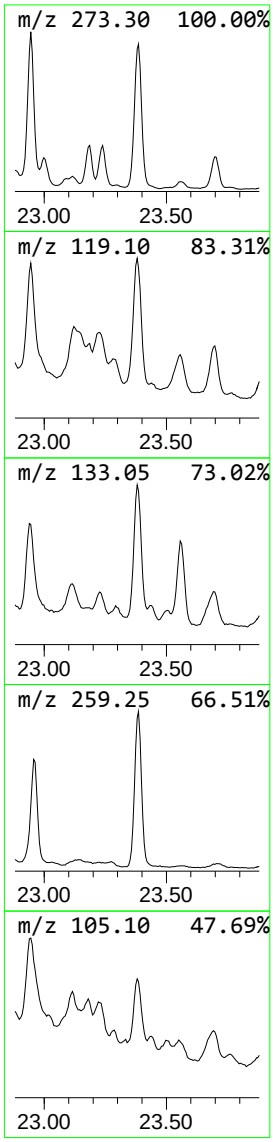
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 unknown23.380 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.380	20.00 ng	8312320	Perylene-d12	24.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3Ah-pyrrolo[3,4-d]isoxazole-3-ca...	274	C13H10N2O5	1010317-17-8	20
2	2-Amino-1-(4-methylphenyl)-4-phe...	315	C20H17N3O	1000479-67-7	20
3	Euparin, TMS derivative	288	C16H20O3Si	1000478-60-9	18
4	N-Methylpiperidino[2,4-b,c]1,2,3...	273	C18H27NO	1000128-54-7	18
5	Terephthalic acid, di(4-fluoro-2...	414	C22H16F2O6	1010415-83-7	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040925\
Data File : BM049874.D
Acq On : 09 Apr 2025 19:01
Operator : RC/JU
Sample : Q1739-01 20X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-LIQUID-20250404

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclohexanone, ...	11.822	15.9	ng	1905960	2	10.569	2393030	20.0
2,4,4,6,6,8,8-H...	12.851	21.6	ng	3041790	3	14.422	2823510	20.0
unknown13.469	13.469	14.7	ng	2073850	3	14.422	2823510	20.0
unknown15.369	15.369	16.5	ng	2324750	3	14.422	2823510	20.0
Benzene, (1-met...	17.075	16.4	ng	9989480	4	17.163	12142200	20.0
Benzene, (1-pro...	17.339	12.9	ng	7840880	4	17.163	12142200	20.0
unknown17.486	17.486	9.5	ng	5740720	4	17.163	12142200	20.0
Benzene, (1-eth...	17.545	23.9	ng	14523000	4	17.163	12142200	20.0
Benzene, (1,1,4...	17.710	24.8	ng	15060800	4	17.163	12142200	20.0
Benzene, (1-met...	17.839	48.2	ng	29244000	4	17.163	12142200	20.0
Benzene, (1-met...	18.551	19.1	ng	11614800	4	17.163	12142200	20.0
unknown21.127	21.127	13.1	ng	11303600	5	21.410	17315700	20.0
unknown21.633	21.633	20.5	ng	17724200	5	21.410	17315700	20.0
unknown21.727	21.727	18.4	ng	15944300	5	21.410	17315700	20.0
1H-Cyclopenta[a...	21.951	17.2	ng	14862200	5	21.410	17315700	20.0
unknown22.051	22.051	21.5	ng	18618800	5	21.410	17315700	20.0
4-(2-Carbamoyl-...	22.298	18.5	ng	16010300	5	21.410	17315700	20.0
unknown22.674	22.674	16.3	ng	14125700	5	21.410	17315700	20.0
1,2,4-Oxadiazol...	22.945	32.3	ng	13412800	6	24.415	8312320	20.0
unknown23.380	23.380	20.0	ng	8312320	6	24.415	8312320	20.0