LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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: BM049963.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.887	317	323	330	rBV	773661	1028863	11.25%	1.126%
2	5.357	397	403	419	rBV	3946941	5552954	60.69%	6.077%
3	5.963	501	506	512	rVB	83540	122663	1.34%	0.134%
4	6.951	663	674	692	rBV	3704411	6004532	65.63%	6.571%
5	7.763	804	812	820	rBV	1543674	2406427	26.30%	2.634%
6	8.922	1001	1009	1020	rBV	2336885	3719874	40.66%	4.071%
7	9.486	1100	1105	1111	rVB	107981	161507	1.77%	0.177%
8	10.557	1280	1287	1294	rBV	1738938	2927382	32.00%	3.204%
9	13.027	1701	1707	1719	rVB	6108274	9149348	100.00%	10.013%
10	14.304	1920	1924	1932	rVB3	83479	185483	2.03%	0.203%
11	14.410	1936	1942	1949	rVV	2663206	3768192	41.19%	4.124%
12	14.627	1976	1979	1986	rVB	69180	102721	1.12%	0.112%
13	15.227	2075	2081	2099	rVB	943133	1710444	18.69%	1.872%
14	15.768	2169	2173	2186	rVB	1054486	1673920	18.30%	1.832%
15	15.898	2190	2195	2204	rVB	3917759	5500093	60.11%	6.019%
16	16.386	2275	2278	2286	rBV3	89037	169358	1.85%	0.185%
17	16.762	2339	2342	2347	rVB2	141156	206121	2.25%	0.226%
18	16.880	2359	2362	2365	rBV2	83216	101852	1.11%	0.111%
19	16.915	2365	2368	2374	rVB3	118426	170240	1.86%	0.186%
20	17.080	2392	2396	2400	rBV2	173379	229603	2.51%	0.251%
21	17.156	2403	2409	2413	rVV	2866232	3960764	43.29%	4.335%
22	17.198	2413	2416	2422	rVB	524140	732194	8.00%	0.801%
23	17.439	2450	2457	2464	rVB2	375078	662942	7.25%	0.726%
24	17.827	2518	2523	2528	rVB	1375943	1835919	20.07%	2.009%
25	18.056	2554	2562	2569	rBV2	2213768	4012055	43.85%	4.391%
26	18.121	2569	2573	2582	rVV	1478491	2449066	26.77%	2.680%
27	18.198	2583	2586	2595	rVB3	171839	378110	4.13%	0.414%
28	18.474	2628	2633	2640	rBV2	822637	1186398	12.97%	1.298%
29	18.598	2651	2654	2662	rVB2	193508	285932	3.13%	0.313%
30	19.215	2754	2759	2766	rVB	1458236	2045804	22.36%	2.239%
31	19.339	2775	2780	2787	rBV	858870	1413455	15.45%	1.547%
32	19.409	2788	2792	2798	rVB3	258735	495578	5.42%	0.542%
33	19.574	2812	2820	2828	rVB	1255391	2033945	22.23%	2.226%
34	19.750	2844	2850	2851	rBV	777298	1126376	12.31%	1.233%
35	19.780	2851	2855	2860	rVB	7708245	9031314	98.71%	9.884%
36	20.074	2901	2905	2917	rVB	1338769	2043811	22.34%	2.237%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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	20.227	2927	2931	2936	rVB3	295092	447415	4.89%	0.490%
38	21.074	3072	3075	3082	rVB4	316354	483642	5.29%	0.529%
39	21.297	3109	3113	3120	rVB	832269	1166753	12.75%	1.277%
40	21.391	3122	3129	3134	rVV2	2907736	5080210	55.53%	5.560%
41	21.433	3134	3136	3148	rVB	618782	860574	9.41%	0.942%
42	24.244	3610	3614	3622	rVB	392969	821435	8.98%	0.899%
43	24.391	3631	3639	3647	rBV	1585645	3930444	42.96%	4.301%

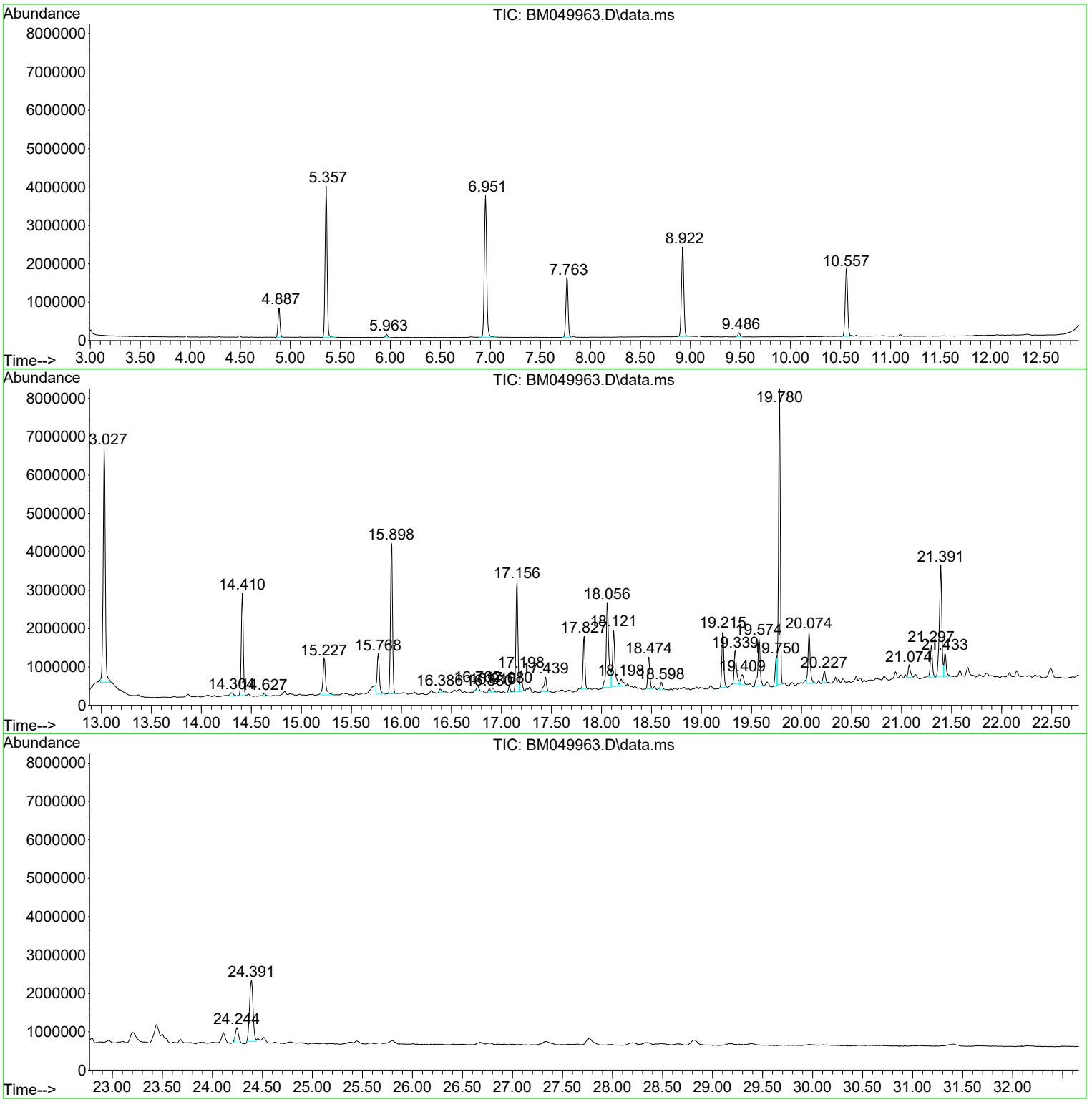
Sum of corrected areas: 91375713

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

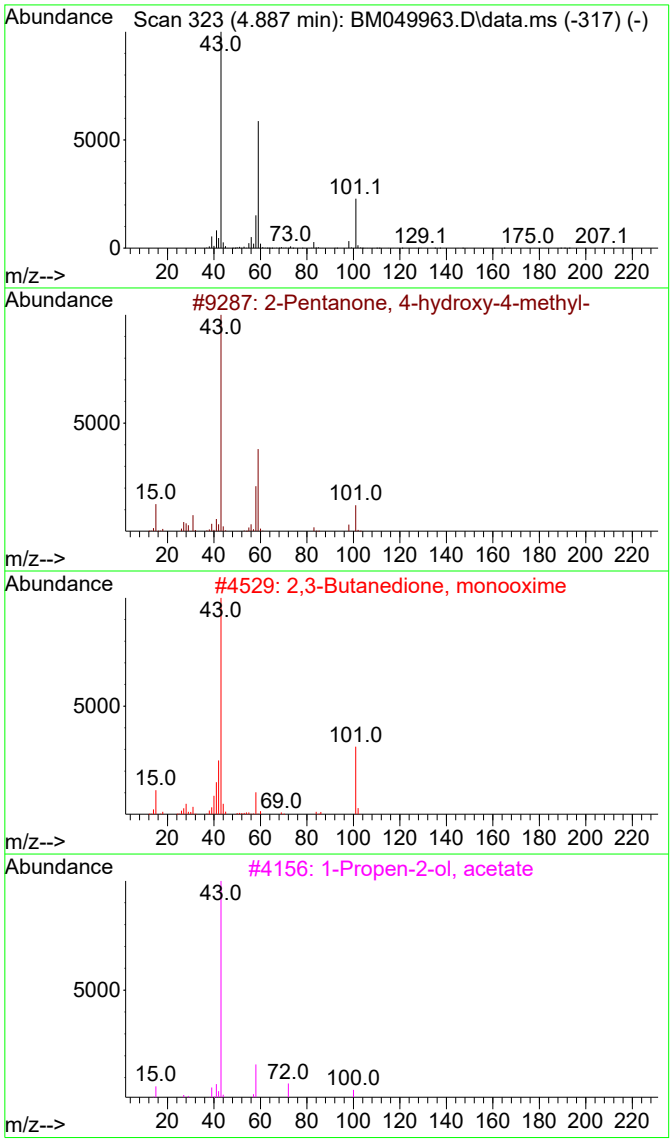
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

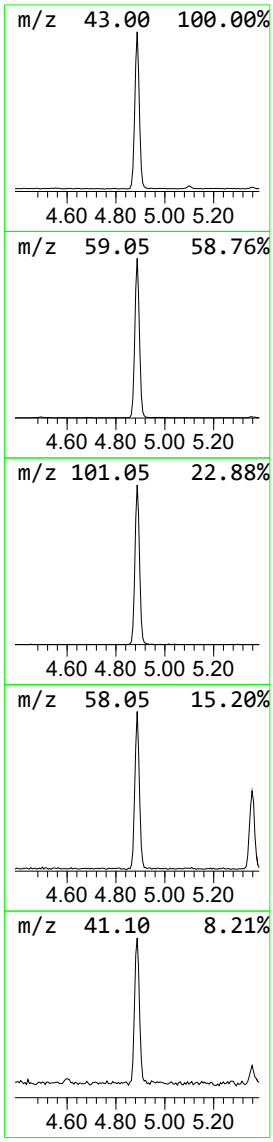
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.887	8.55 ng	1028860	1,4-Dichlorobenzene-d4	7.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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

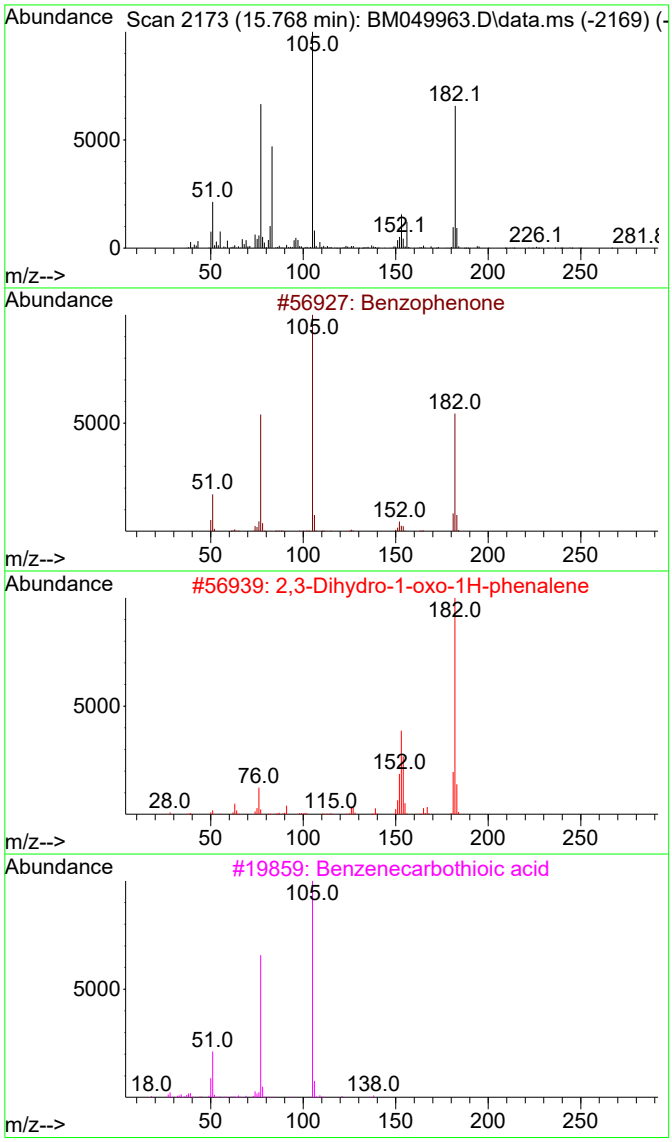
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

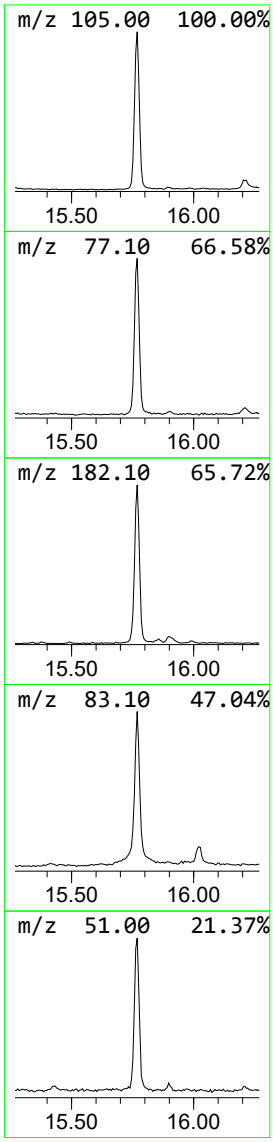
****

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.768	8.88 ng	1673920	Acenaphthene-d10	14.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	2,3-Dihydro-1-oxo-1H-phenalene	182	C13H10O	000518-85-4	30
3	Benzenecarbothioic acid	138	C7H6OS	000098-91-9	30
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	27
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

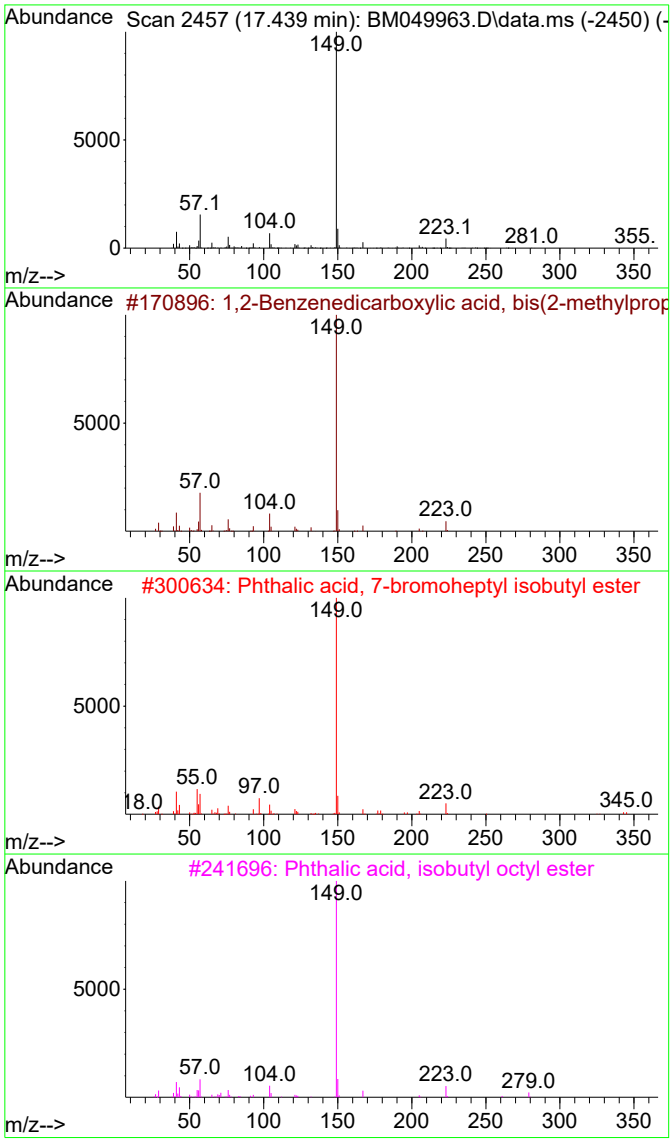
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

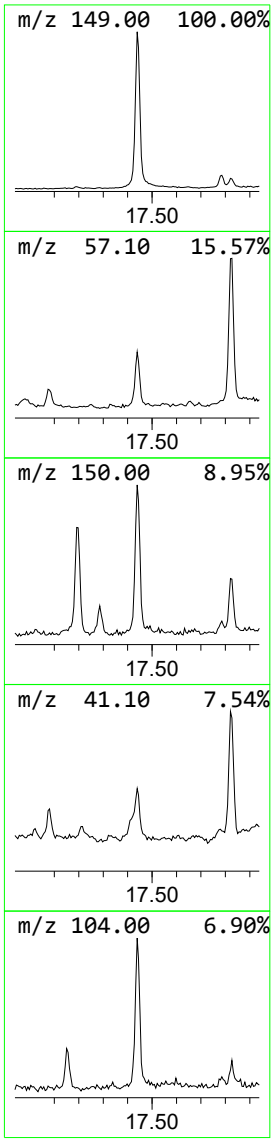
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,2-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.439	3.35 ng	662942	Phenanthrene-d10	17.156

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2	Phthalic acid, 7-bromoheptyl iso...	398	C19H27BrO4	1000415-51-7	86
3	Phthalic acid, isobutyl octyl ester	334	C20H30O4	1010309-04-5	83
4	Phthalic acid, isobutyl 2-propyl...	334	C20H30O4	1000377-91-9	78
5	Phthalic acid, isobutyl 6-methyl...	334	C20H30O4	1000377-95-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

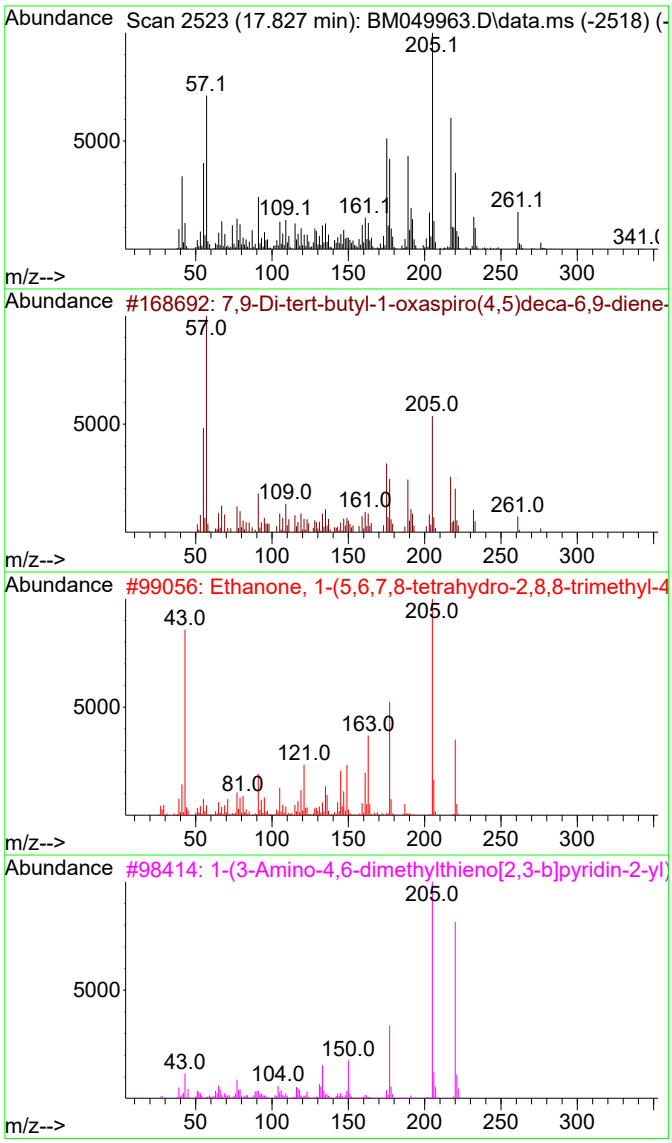
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

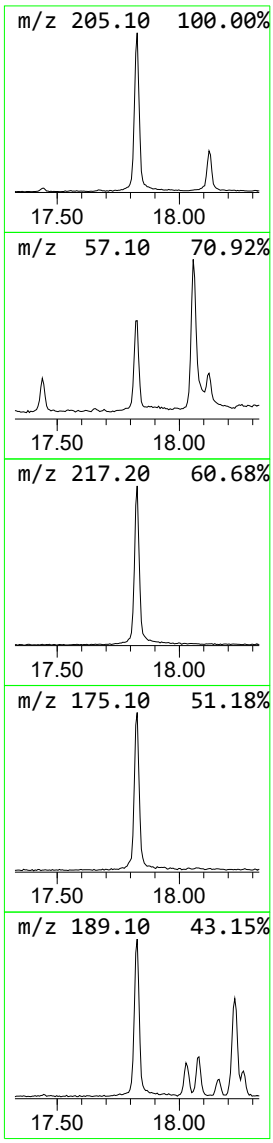
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.827	9.27 ng	1835920	Phenanthrene-d10	17.156

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	64
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	50
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	42
5	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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

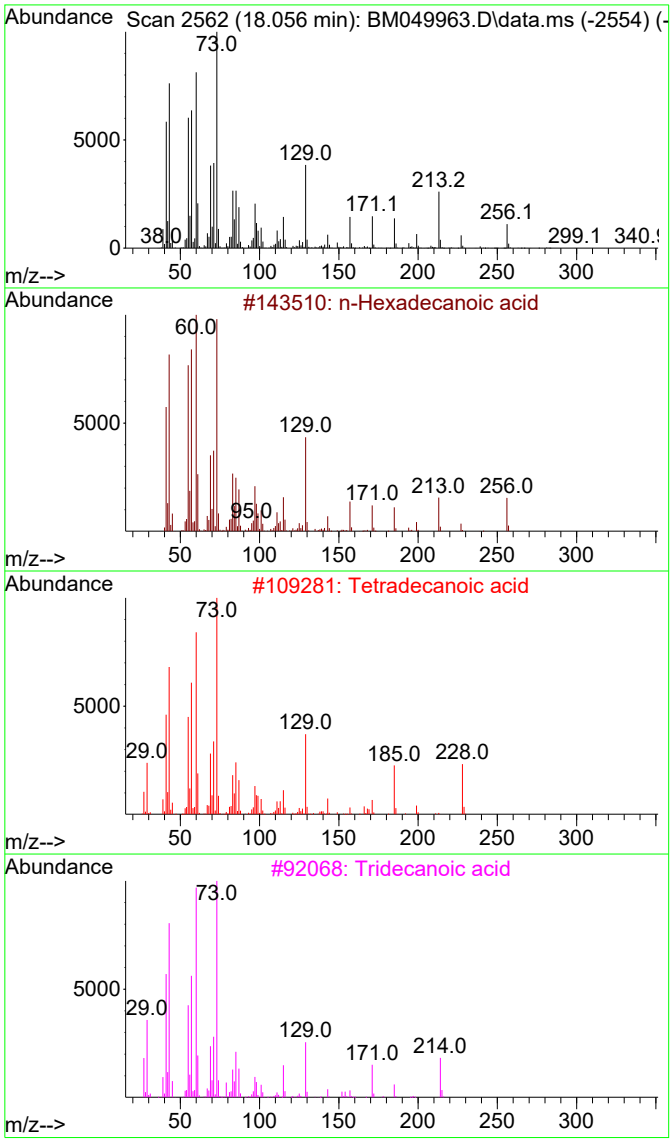
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

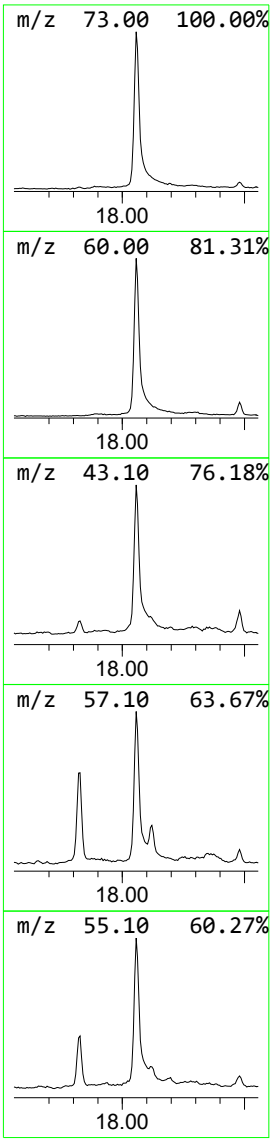
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.056	20.26 ng	4012060	Phenanthrene-d10	17.156

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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

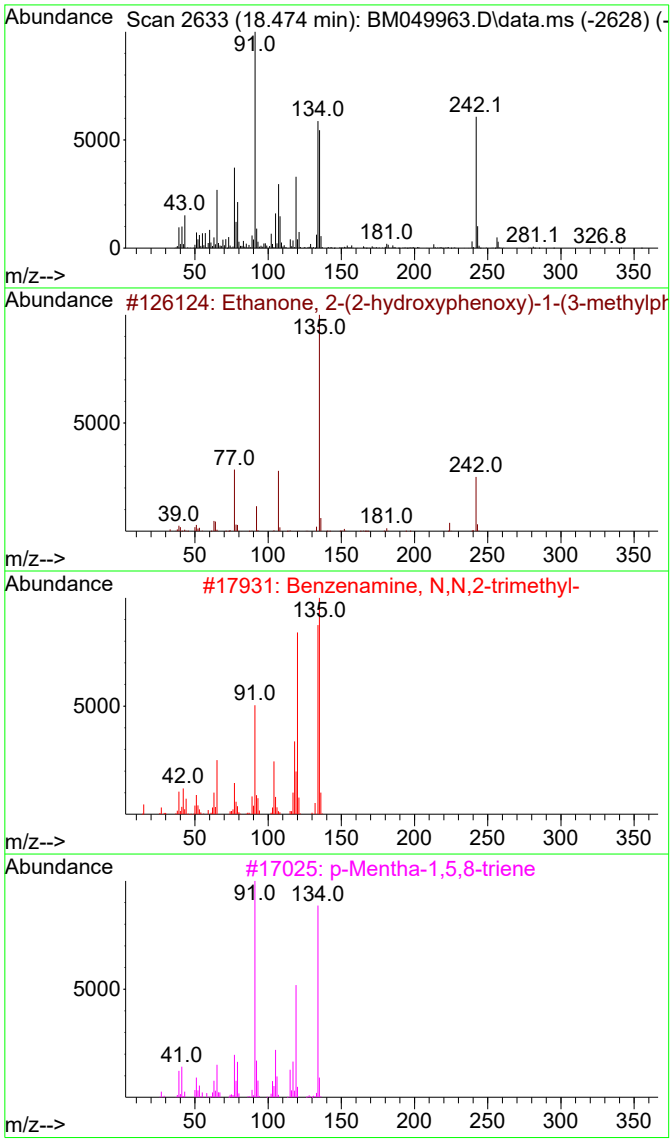
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

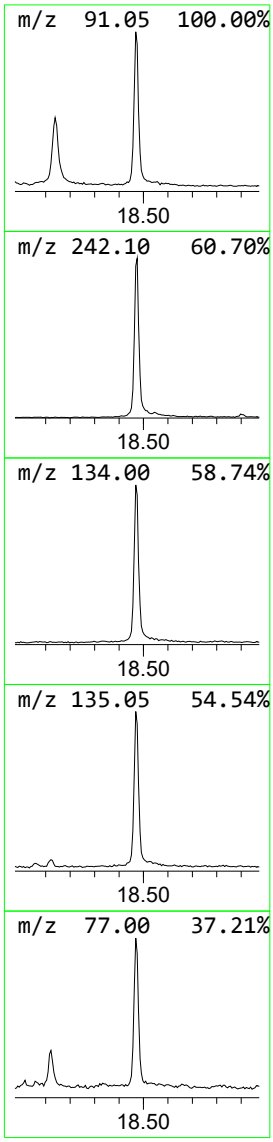
****

Peak Number 6 unknown18.474 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.474	5.99 ng	1186400	Phenanthrene-d10	17.156

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 2-(2-hydroxyphenoxy)-1...	242	C15H14O3	1010269-83-9	43
2	Benzenamine, N,N,2-trimethyl-	135	C9H13N	000609-72-3	38
3	p-Mentha-1,5,8-triene	134	C10H14	021195-59-5	38
4	N-Benzylformamide	135	C8H9NO	006343-54-0	30
5	Carbonic acid, bis(4-methylpheny...	242	C15H14O3	000621-02-3	30





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Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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

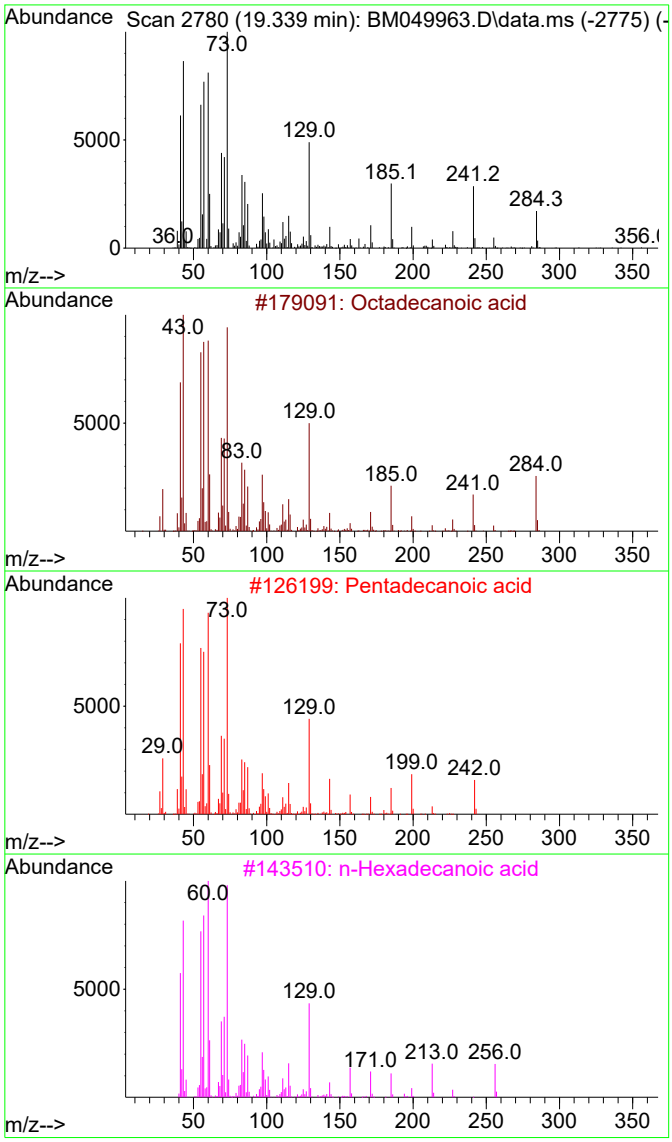
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

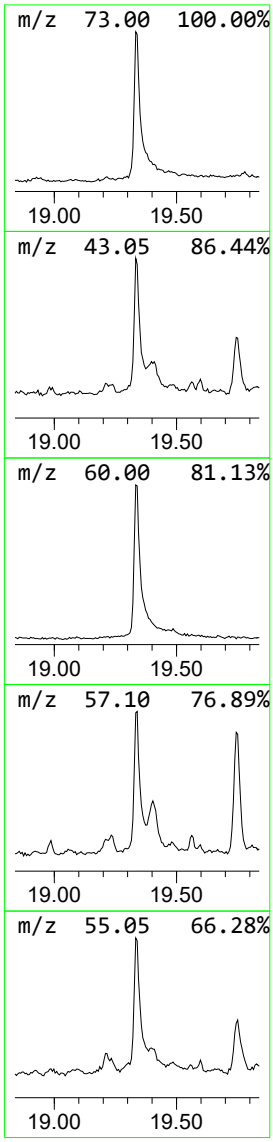
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	5.56 ng	1413460	Chrysene-d12	21.391

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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

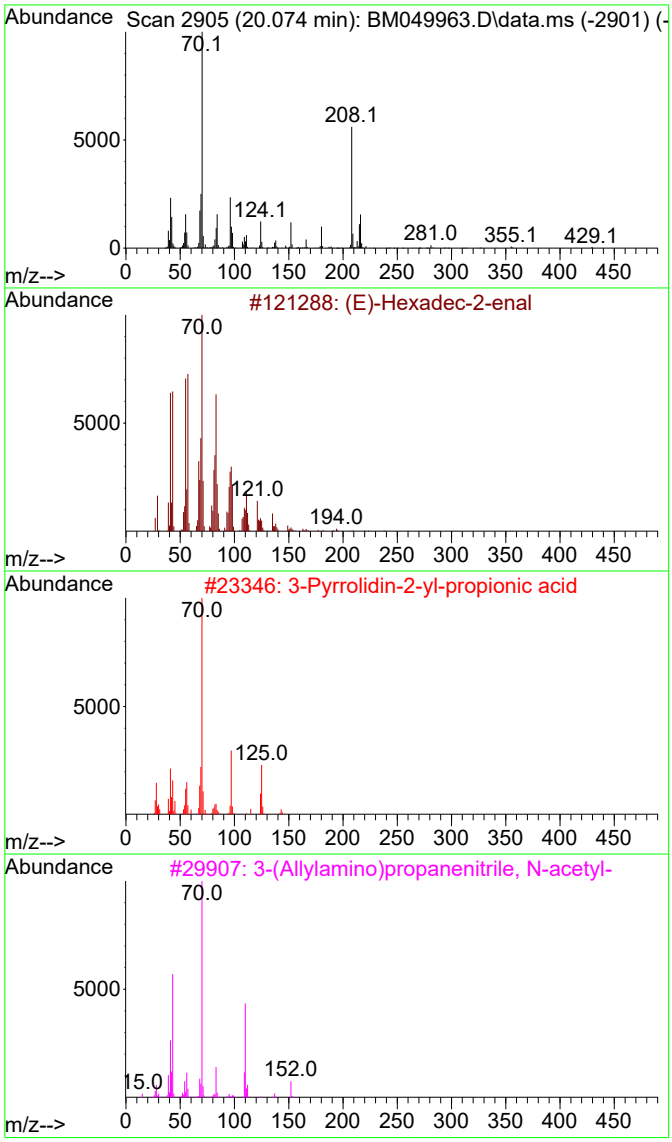
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

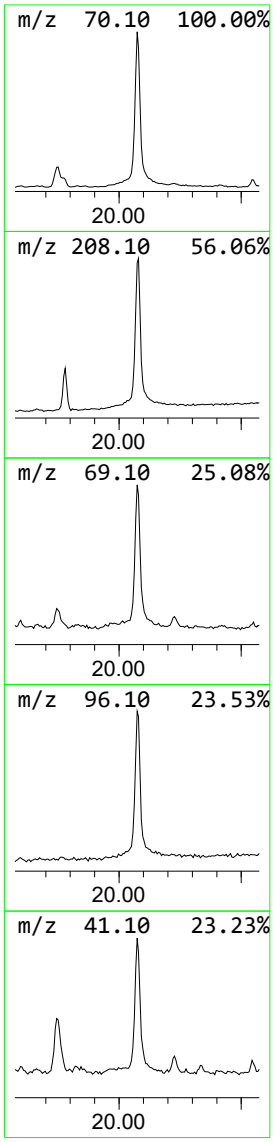
****

Peak Number 8 unknown20.074 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.074	8.05 ng	2043810	Chrysene-d12	21.391

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-2-enal	238	C16H30O	022644-96-8	32
2	3-Pyrrolidin-2-yl-propionic acid	143	C7H13NO2	1000193-88-0	17
3	3-(Allylamino)propanenitrile, N-...	152	C8H12N2O	1000475-61-4	17
4	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	17
5	1-Decene, 3,3,4-trimethyl-	182	C13H26	049622-17-5	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041825\
Data File : BM049963.D
Acq On : 18 Apr 2025 13:10
Operator : RC/JU
Sample : Q1825-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-9

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
2-Pentanone, 4-...	4.887	8.6	ng	1028860	1	7.769	2406430	20.0
Benzophenone	15.768	8.9	ng	1673920	3	14.410	3768190	20.0
1,2-Benzenedica...	17.439	3.4	ng	662942	4	17.156	3960760	20.0
7,9-Di-tert-but...	17.827	9.3	ng	1835920	4	17.156	3960760	20.0
n-Hexadecanoic ...	18.056	20.3	ng	4012060	4	17.156	3960760	20.0
unknown18.474	18.474	6.0	ng	1186400	4	17.156	3960760	20.0
Octadecanoic acid	19.339	5.6	ng	1413460	5	21.391	5080210	20.0
unknown20.074	20.074	8.1	ng	2043810	5	21.391	5080210	20.0