LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020507.D
Acq On : 04 Jun 2024 22:39
Operator : MA/JU
Sample : P2687-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 72-11998

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_P\Methods\8270E-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020507.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	4	9	22	rVB	2330674	3397881	33.78%	4.114%
2	3.558	93	97	106	rBV	247772	340622	3.39%	0.412%
3	4.934	323	331	336	rBV	75318	113506	1.13%	0.137%
4	5.375	399	406	419	rBV	2968987	4457417	44.31%	5.396%
5	6.934	662	671	683	rBV	3020098	4770460	47.42%	5.775%
6	7.764	805	812	819	rBV	1021789	1640056	16.30%	1.985%
7	8.905	996	1006	1015	rBV	1792442	3065686	30.47%	3.711%
8	9.463	1095	1101	1107	rVB	84520	129947	1.29%	0.157%
9	10.534	1275	1283	1290	rBV	1361549	2365727	23.52%	2.864%
10	11.269	1400	1408	1415	rBV	178320	314311	3.12%	0.381%
11	12.999	1691	1702	1709	rBV	4703704	7213874	71.71%	8.733%
12	14.387	1928	1938	1945	rBV	2018098	3191037	31.72%	3.863%
13	15.904	2189	2196	2207	rBV	3583591	5188800	51.58%	6.282%
14	17.198	2409	2416	2420	rBV	2441928	3709487	36.87%	4.491%
15	17.240	2420	2423	2430	rVV	867650	1262534	12.55%	1.528%
16	17.334	2434	2439	2445	rVB	75908	125625	1.25%	0.152%
17	17.616	2483	2487	2492	rVB	85760	116375	1.16%	0.141%
18	18.110	2564	2571	2574	rBV	113023	184816	1.84%	0.224%
19	18.151	2574	2578	2587	rVB2	534573	795653	7.91%	0.963%
20	18.292	2598	2602	2607	rBV2	127617	217760	2.16%	0.264%
21	18.516	2635	2640	2650	rBV5	165431	335821	3.34%	0.407%
22	18.634	2656	2660	2662	rBV	76821	115794	1.15%	0.140%
23	18.663	2662	2665	2672	rVB	176000	273528	2.72%	0.331%
24	19.057	2727	2732	2738	rBV3	65123	140557	1.40%	0.170%
25	19.198	2753	2756	2763	rVB2	85724	136857	1.36%	0.166%
26	19.328	2773	2778	2786	rBV	1919117	2868686	28.52%	3.473%
27	19.481	2800	2804	2809	rVB2	209286	313423	3.12%	0.379%
28	19.704	2831	2842	2850	rBV2	1380308	2452770	24.38%	2.969%
29	19.928	2872	2880	2888	rVB	6863520	10060093	100.00%	12.179%
30	20.051	2896	2901	2902	rBV2	80280	111504	1.11%	0.135%
31	20.222	2928	2930	2938	rVB	190598	273540	2.72%	0.331%
32	20.333	2945	2949	2952	rVB	88977	111427	1.11%	0.135%
33	20.392	2955	2959	2963	rVB3	89625	139297	1.38%	0.169%
34	21.010	3061	3064	3074	rVB	160488	287279	2.86%	0.348%
35	21.257	3103	3106	3110	rBV	115623	159182	1.58%	0.193%
36	21.298	3110	3113	3115	rVV	122052	171278	1.70%	0.207%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020507.D
Acq On : 04 Jun 2024 22:39
Operator : MA/JU
Sample : P2687-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11998

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_P\Methods\8270E-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.339	3116	3120	3132	rVB4	541094	1186043	11.79%	1.436%
38	21.592	3159	3163	3164	rBV	110575	132880	1.32%	0.161%
39	21.651	3164	3173	3177	rVV3	2506598	5338159	53.06%	6.462%
40	21.692	3177	3180	3190	rVB	787834	1320799	13.13%	1.599%
41	22.598	3331	3334	3335	rBV	153841	164175	1.63%	0.199%
42	22.963	3389	3396	3406	rBV	2298512	4704845	46.77%	5.696%
43	23.939	3555	3562	3570	rBV2	576867	1782429	17.72%	2.158%
44	24.216	3603	3609	3611	rBV4	130039	288333	2.87%	0.349%
45	24.257	3612	3616	3633	rVB2	314374	876641	8.71%	1.061%
46	24.686	3683	3689	3705	rVB2	391819	1062623	10.56%	1.286%
47	24.833	3708	3714	3726	rVB2	402941	1105695	10.99%	1.339%
48	24.998	3733	3742	3752	rBV	1638557	4087387	40.63%	4.948%

Sum of corrected areas: 82602619

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Instrument :
BNA_P
ClientSampleId :
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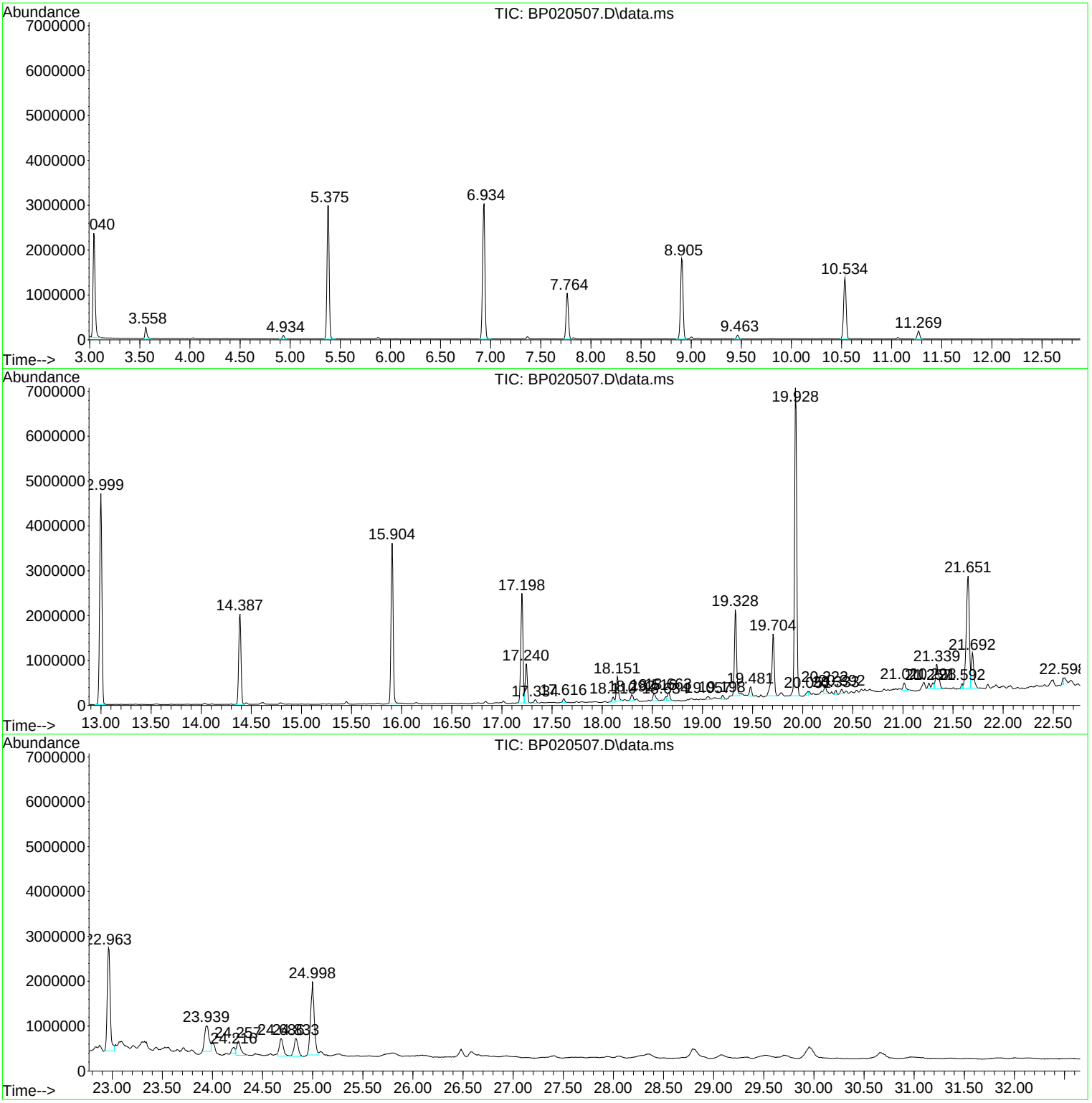
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020507.D
Acq On : 04 Jun 2024 22:39
Operator : MA/JU
Sample : P2687-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

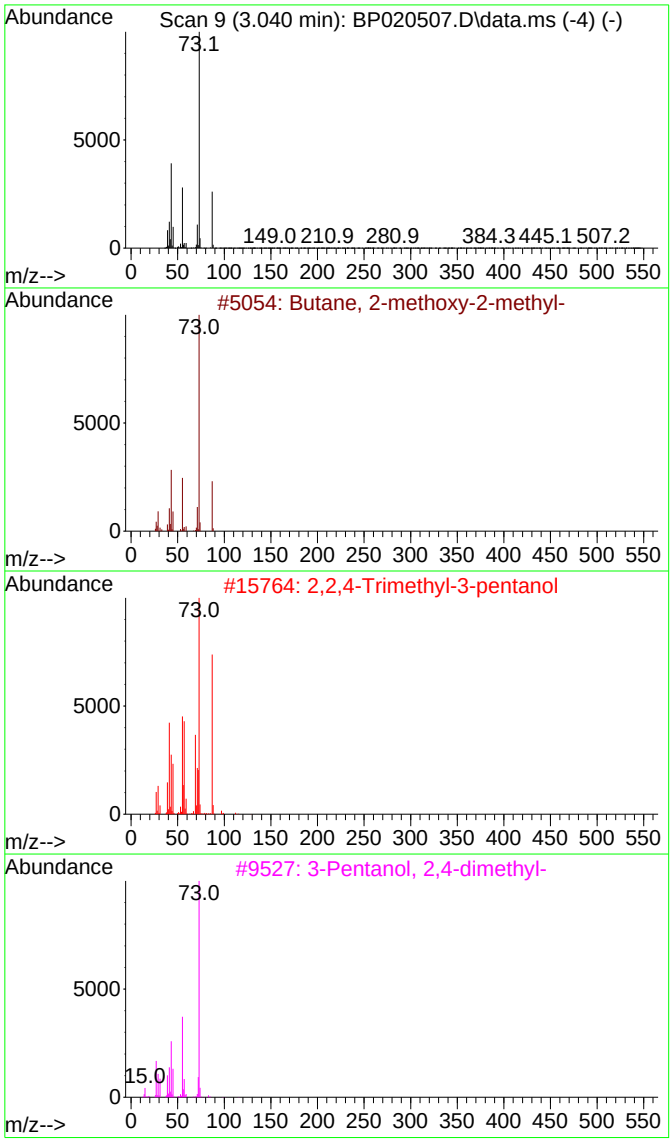
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

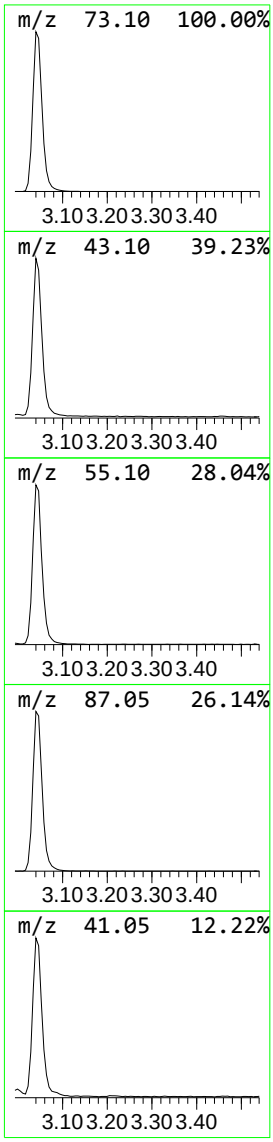
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.040	41.44 ng	3397880	1,4-Dichlorobenzene-d4	7.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

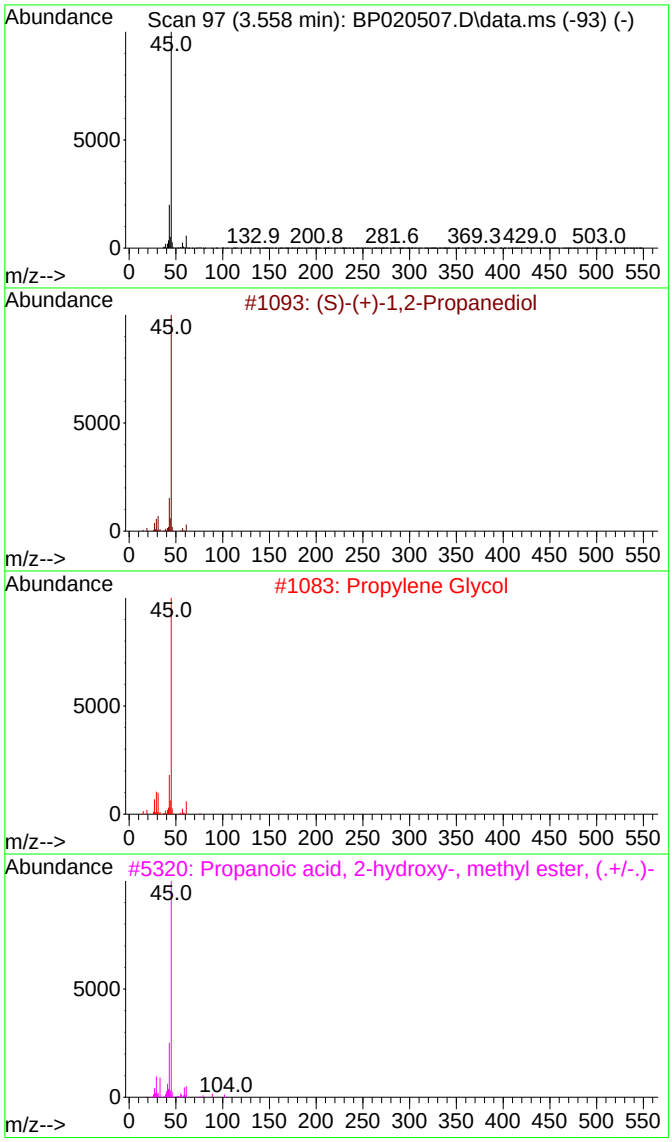
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

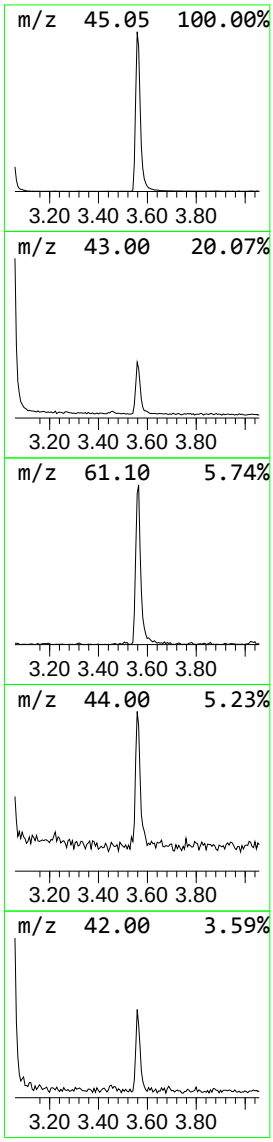
****

Peak Number 2 unknown3.558 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.558	4.15 ng	340622	1,4-Dichlorobenzene-d4	7.764

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	43
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
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Sample : P2687-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

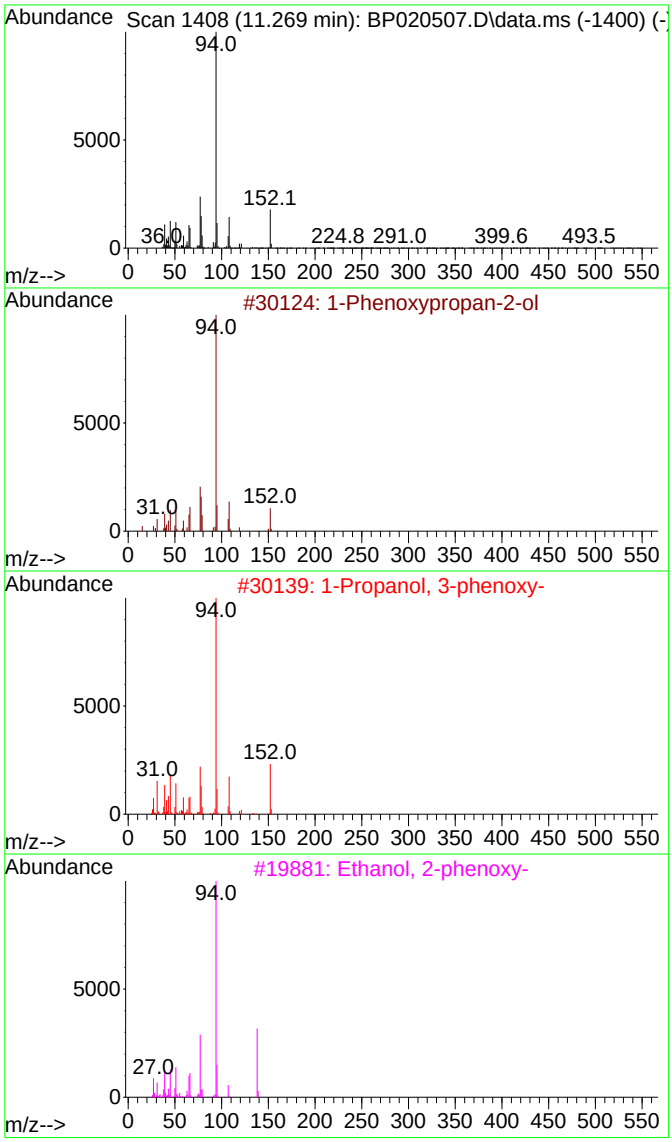
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

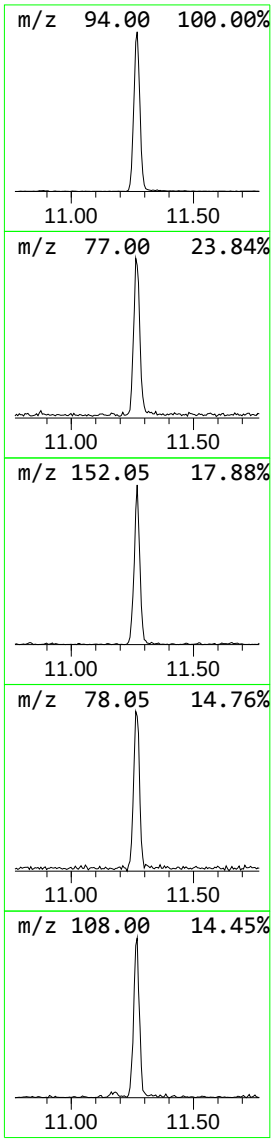
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	2.66 ng	314311	Naphthalene-d8	10.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Sample : P2687-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

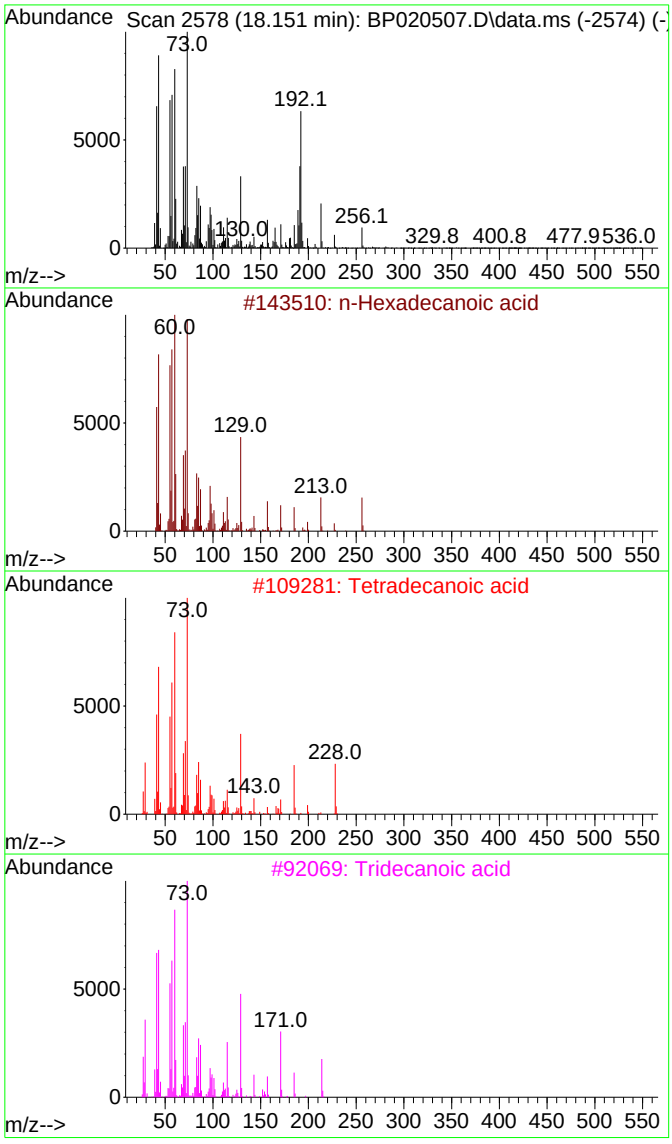
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

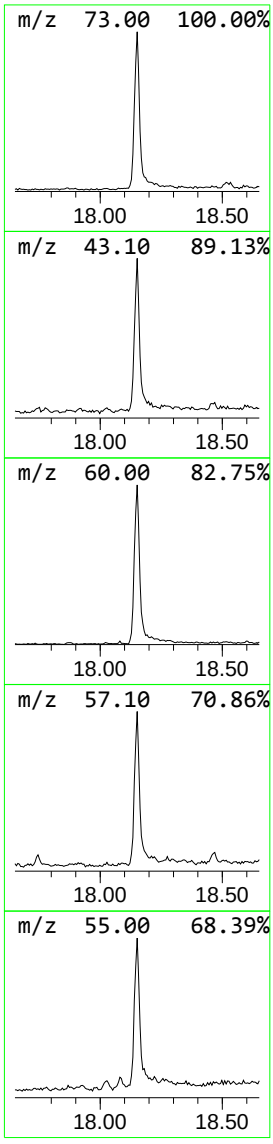
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	4.29 ng	795653	Phenanthrene-d10	17.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	74





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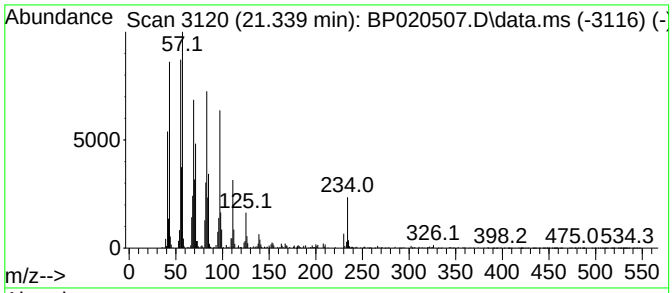
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

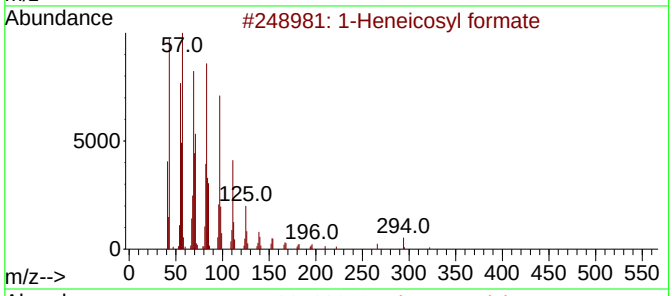
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

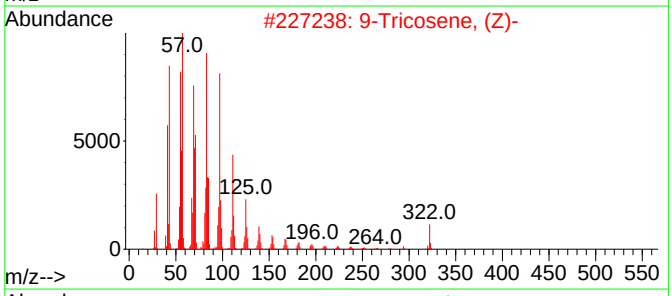
****
Peak Number 5 1-Heneicosyl formate Concentration Rank 4

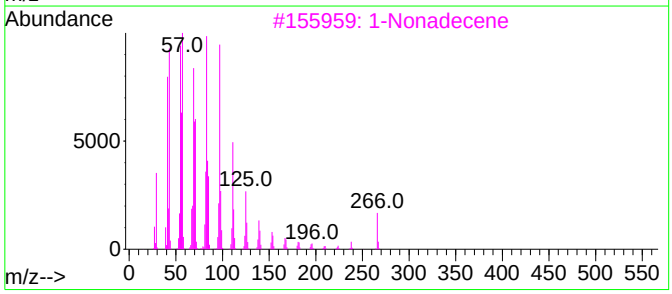
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.339	4.44 ng	1186040	Chrysene-d12	21.651

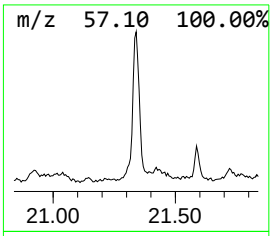
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	99
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	98
3	1-Nonadecene	266	C19H38	018435-45-5	95
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93

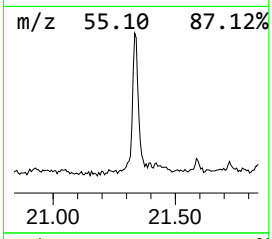


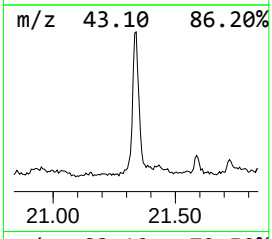


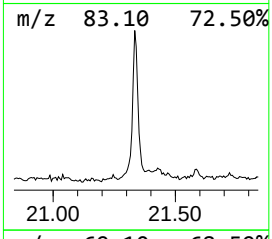


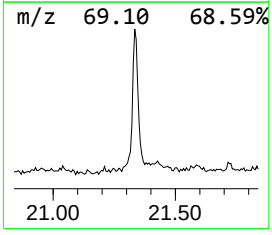












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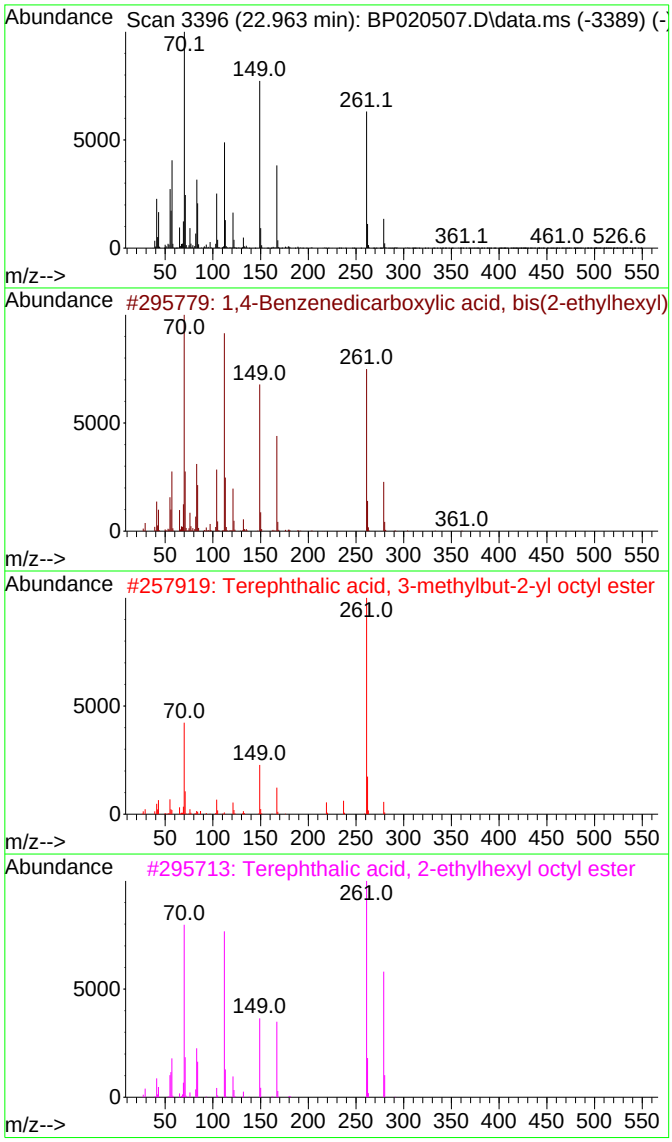
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

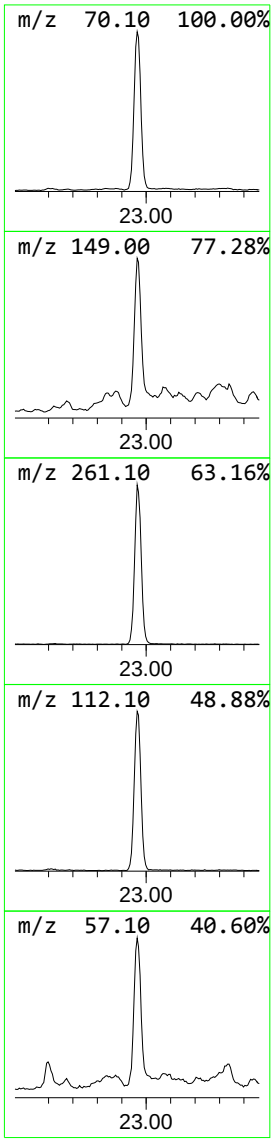
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.963	17.63 ng	4704850	Chrysene-d12	21.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
3	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	49
4	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
5	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020507.D
Acq On : 04 Jun 2024 22:39
Operator : MA/JU
Sample : P2687-07
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

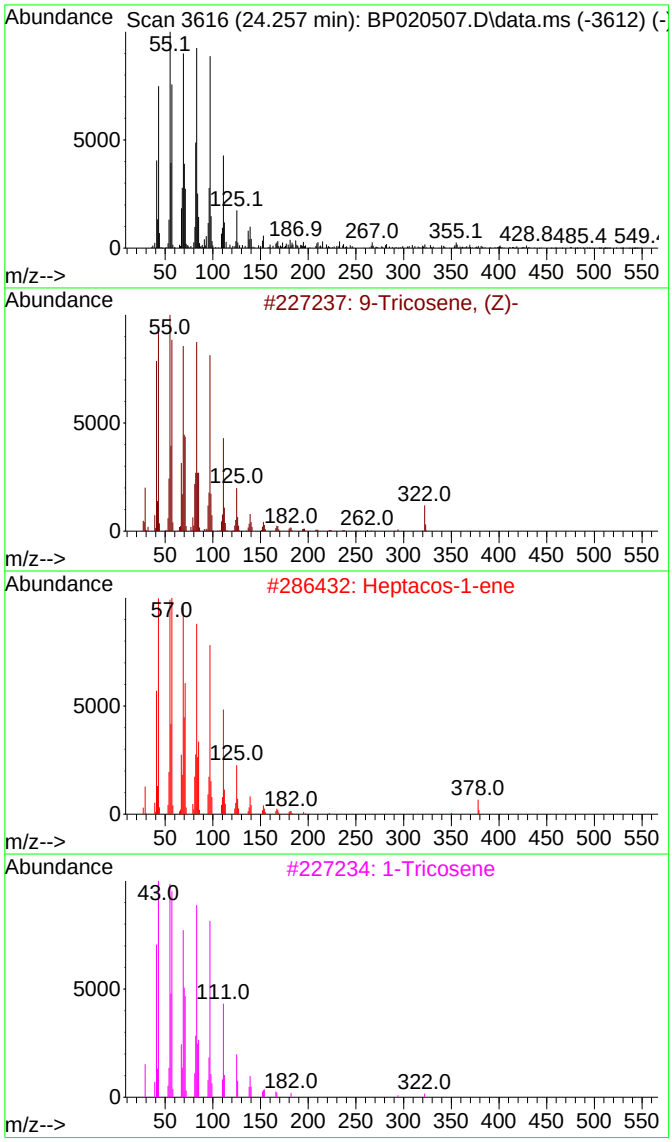
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

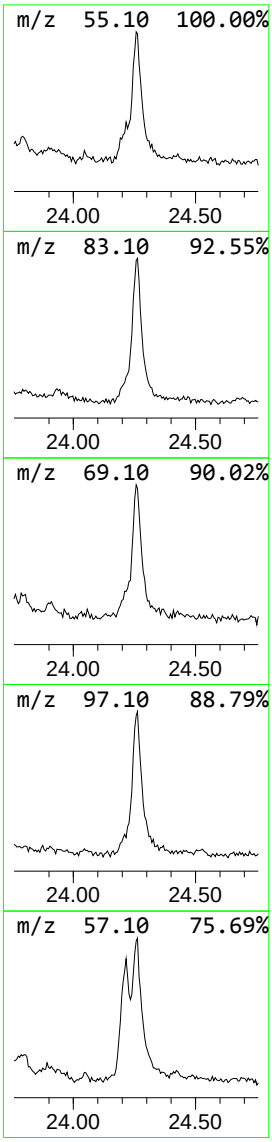
****

Peak Number 7 9-Tricosene, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.257	4.29 ng	876641	Perylene-d12	24.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
2	Heptacos-1-ene	378	C27H54	015306-27-1	90
3	1-Tricosene	322	C23H46	018835-32-0	89
4	2-Methyl-2-docosene	322	C23H46	1000131-16-9	89
5	Cyclooctacosane	392	C28H56	000297-24-5	89





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020507.D
Acq On : 04 Jun 2024 22:39
Operator : MA/JU
Sample : P2687-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

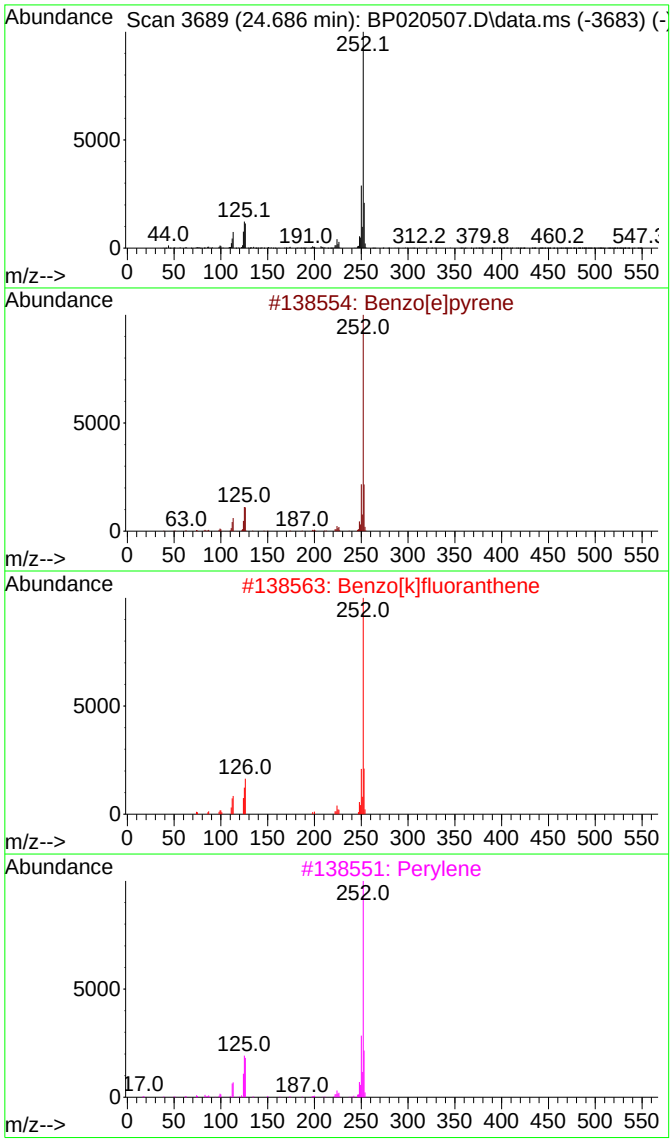
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

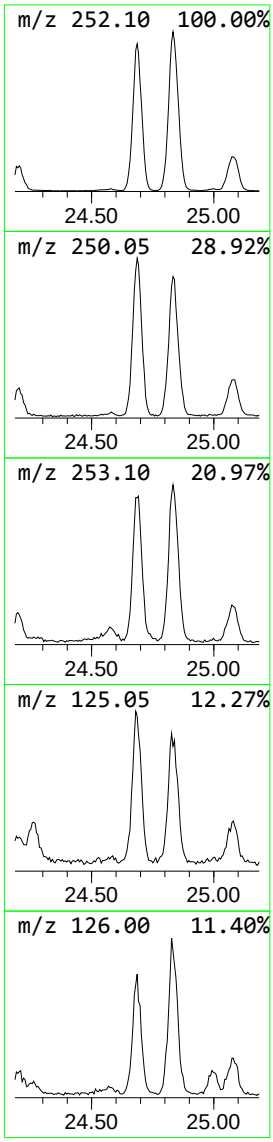
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.686	5.20 ng	1062620	Perylene-d12	24.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020507.D
Acq On : 04 Jun 2024 22:39
Operator : MA/JU
Sample : P2687-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11998

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.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
Butane, 2-metho...	3.040	41.4	ng	3397880	1	7.764	1640060	20.0
unknown3.558	3.558	4.2	ng	340622	1	7.764	1640060	20.0
1-Phenoxypropan...	11.269	2.7	ng	314311	2	10.534	2365730	20.0
n-Hexadecanoic ...	18.151	4.3	ng	795653	4	17.198	3709490	20.0
1-Heneicosyl fo...	21.339	4.4	ng	1186040	5	21.651	5338160	20.0
1,4-Benzenedica...	22.963	17.6	ng	4704850	5	21.651	5338160	20.0
9-Tricosene, (Z)-	24.257	4.3	ng	876641	6	24.998	4087390	20.0
Benzo[e]pyrene	24.686	5.2	ng	1062620	6	24.998	4087390	20.0