LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021618.D
Acq On : 22 Aug 2024 17:58
Operator : RC/JU
Sample : P3518-21
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OU4-TS-11-080724

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-BP081324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021618.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	20	rVB	2356825	3221551	38.25%	4.379%
2	3.546	91	95	107	rVB	253223	365570	4.34%	0.497%
3	4.940	325	332	339	rVB	210167	318403	3.78%	0.433%
4	5.399	402	410	422	rBV	3842029	5758590	68.37%	7.828%
5	6.964	668	676	692	rBV	3882074	6206972	73.69%	8.437%
6	7.393	744	749	764	rVB	117230	193361	2.30%	0.263%
7	7.799	811	818	825	rBV	1265224	1981297	23.52%	2.693%
8	8.940	1002	1012	1024	rBV	2157701	3796187	45.07%	5.160%
9	10.581	1283	1291	1307	rBV	1578044	2816704	33.44%	3.829%
10	11.328	1410	1418	1433	rBV	312293	654525	7.77%	0.890%
11	13.057	1703	1712	1725	rBV	4116369	5975067	70.94%	8.122%
12	14.446	1941	1948	1957	rBV	2435088	3722796	44.20%	5.060%
13	14.681	1978	1988	1993	rBV	253752	622009	7.38%	0.845%
14	15.963	2199	2206	2216	rBV	3777281	6255101	74.26%	8.502%
15	17.257	2419	2426	2430	rBV	2973462	4522595	53.69%	6.147%
16	17.298	2430	2433	2441	rVV	286029	394958	4.69%	0.537%
17	17.392	2443	2449	2455	rVB	67143	150510	1.79%	0.205%
18	17.975	2545	2548	2554	rVB	114573	131302	1.56%	0.178%
19	18.157	2573	2579	2583	rBV4	45963	99096	1.18%	0.135%
20	18.210	2583	2588	2596	rBV2	531988	814070	9.66%	1.107%
21	18.363	2611	2614	2619	rBV2	67077	98637	1.17%	0.134%
22	18.522	2636	2641	2646	rBV3	97271	169830	2.02%	0.231%
23	19.198	2752	2756	2762	rVB6	103515	169826	2.02%	0.231%
24	19.386	2783	2788	2795	rBV	1147042	1450535	17.22%	1.972%
25	19.533	2810	2813	2819	rBV3	166458	238291	2.83%	0.324%
26	19.763	2843	2852	2859	rBV	908618	1572626	18.67%	2.138%
27	19.986	2885	2890	2896	rBV	6478492	8423032	100.00%	11.449%
28	20.281	2937	2940	2946	rVB3	132261	200893	2.39%	0.273%
29	20.392	2956	2959	2963	rBV	117760	155510	1.85%	0.211%
30	21.392	3126	3129	3136	rVB	447593	635629	7.55%	0.864%
31	21.722	3178	3185	3191	rBV2	2992068	5625187	66.78%	7.646%
32	21.769	3191	3193	3204	rVB	404607	595382	7.07%	0.809%
33	24.333	3624	3629	3637	rVB	546396	1139302	13.53%	1.549%
34	25.151	3759	3768	3778	rVB	1965185	5092999	60.47%	6.923%

Sum of corrected areas: 73568343

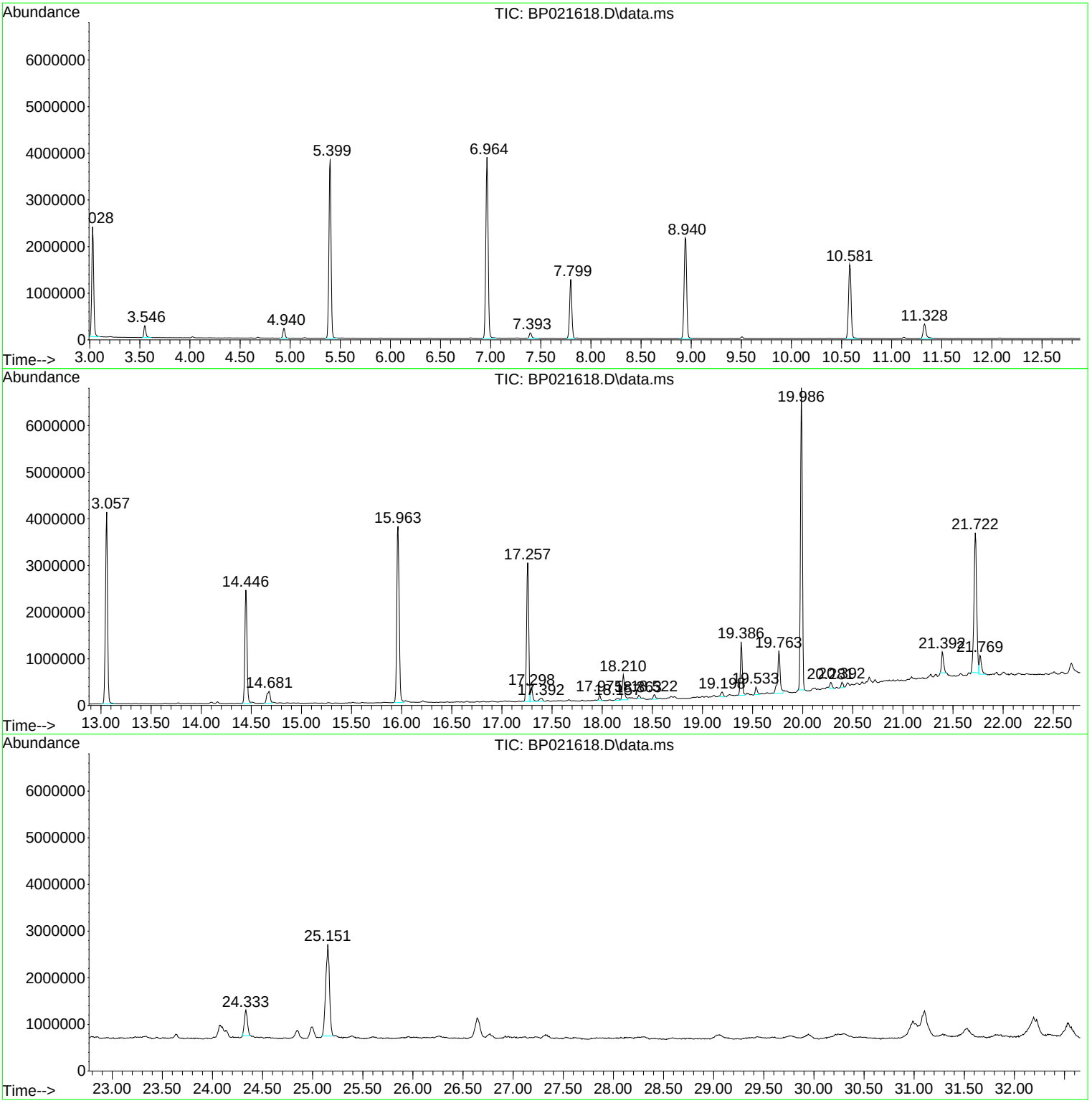
Instrument :
BNA_P
ClientSampleId :
OU4-TS-11-080724

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021618.D
Acq On : 22 Aug 2024 17:58
Operator : RC/JU
Sample : P3518-21
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OU4-TS-11-080724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

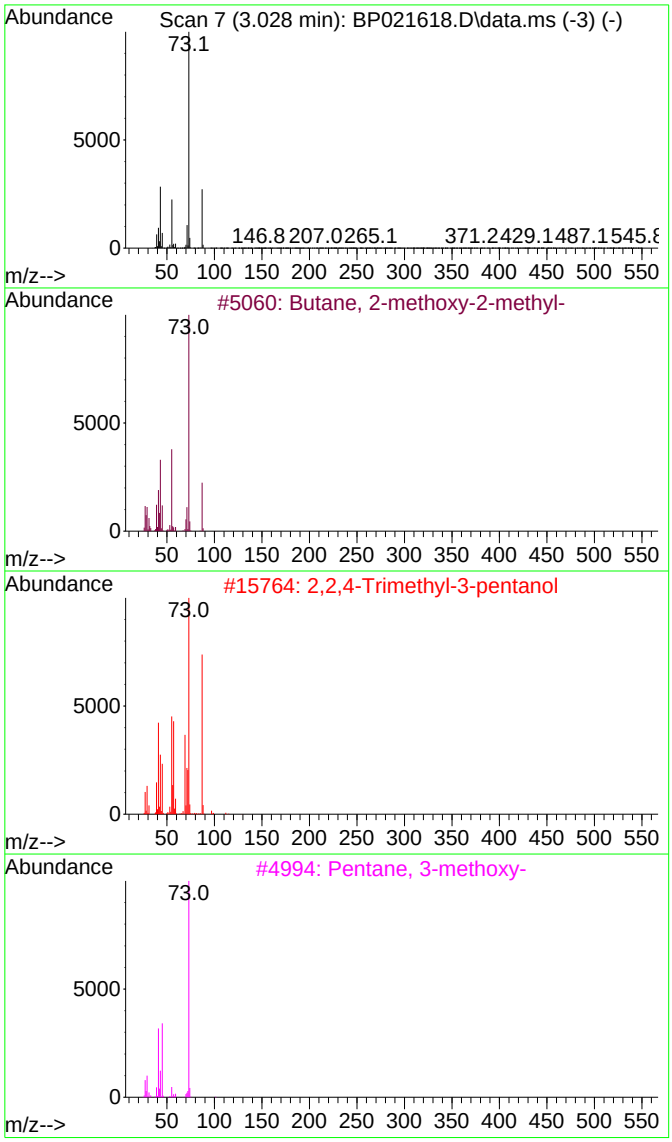
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

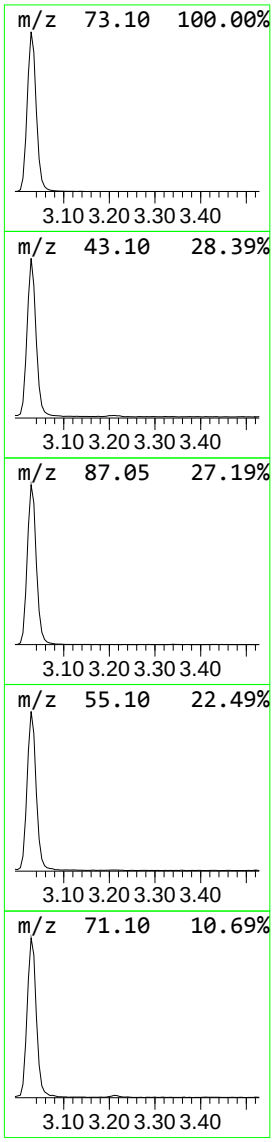
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	32.52 ng	3221550	1,4-Dichlorobenzene-d4	7.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Data File : BP021618.D
Acq On : 22 Aug 2024 17:58
Operator : RC/JU
Sample : P3518-21
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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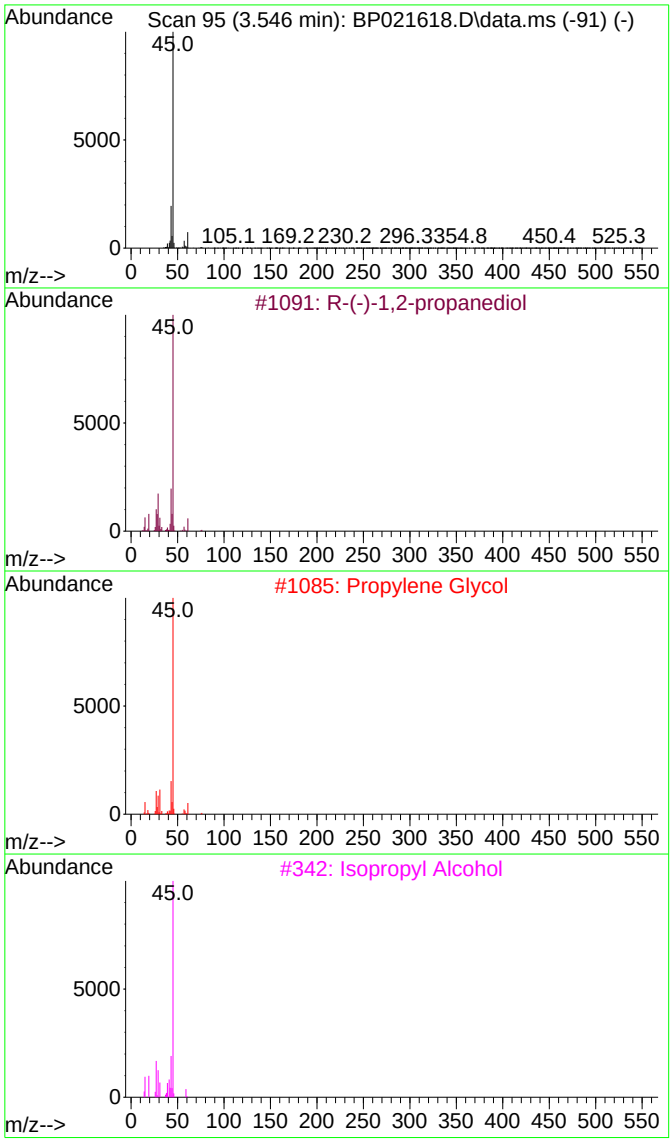
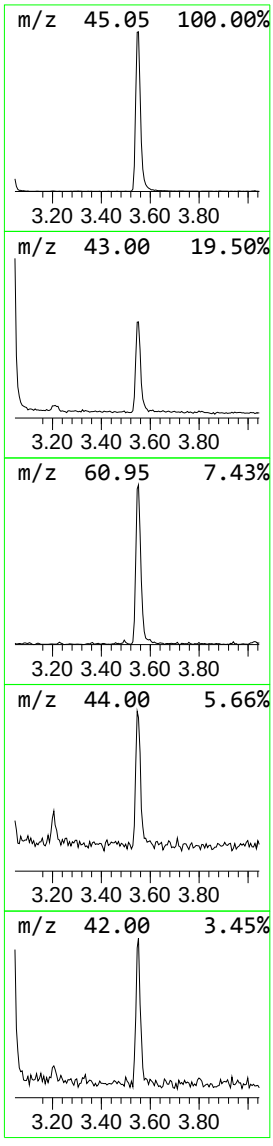
Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	3.69 ng	365570	1,4-Dichlorobenzene-d4	7.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
2	Propylene Glycol	76	C3H8O2	000057-55-6	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	40
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	2-Methoxyisopropyl cyanoacetate	157	C7H11NO3	032804-79-8	9





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Instrument :
BNA_P
ClientSampleId :
OU4-TS-11-080724

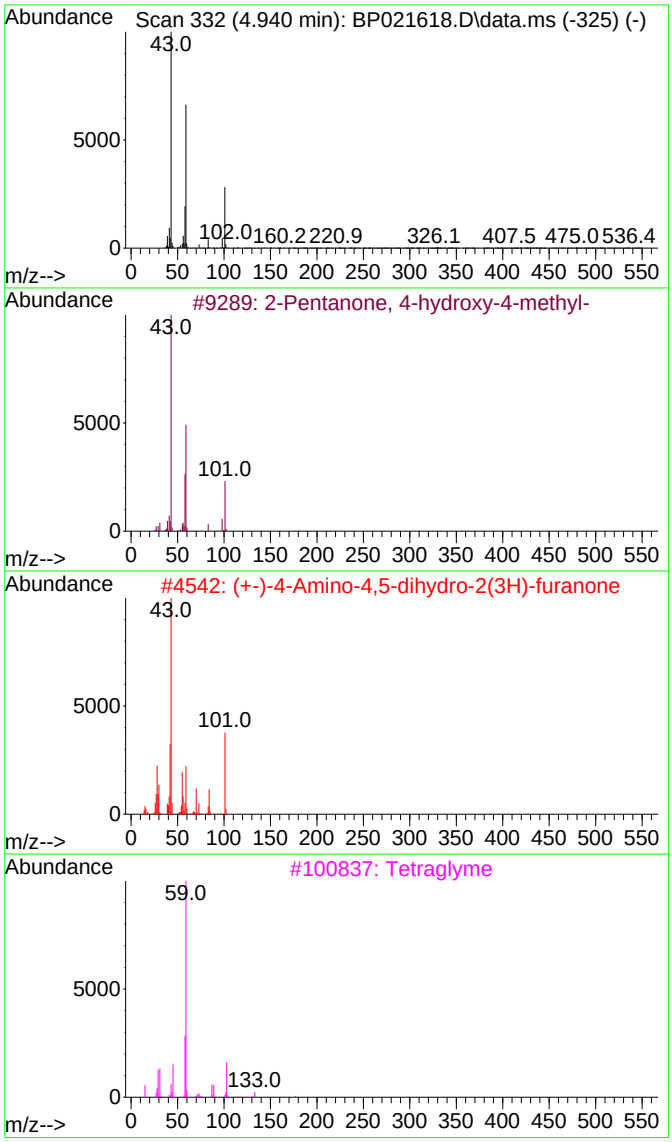
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

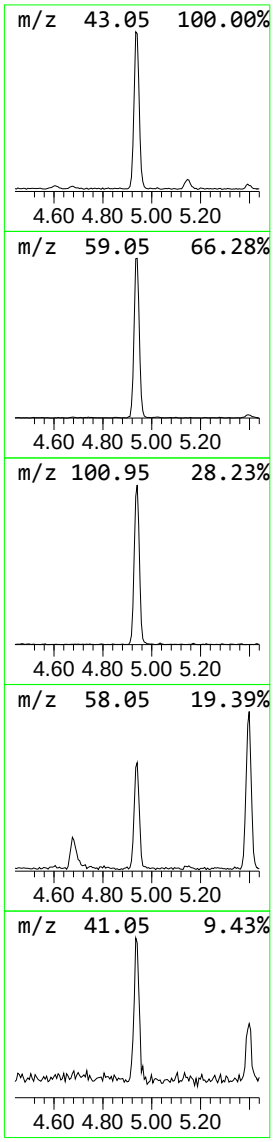
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	3.21 ng	318403	1,4-Dichlorobenzene-d4	7.799

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Tetraglyme	222	C10H22O5	000143-24-8	28
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5	2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	25





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Data File : BP021618.D
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Operator : RC/JU
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BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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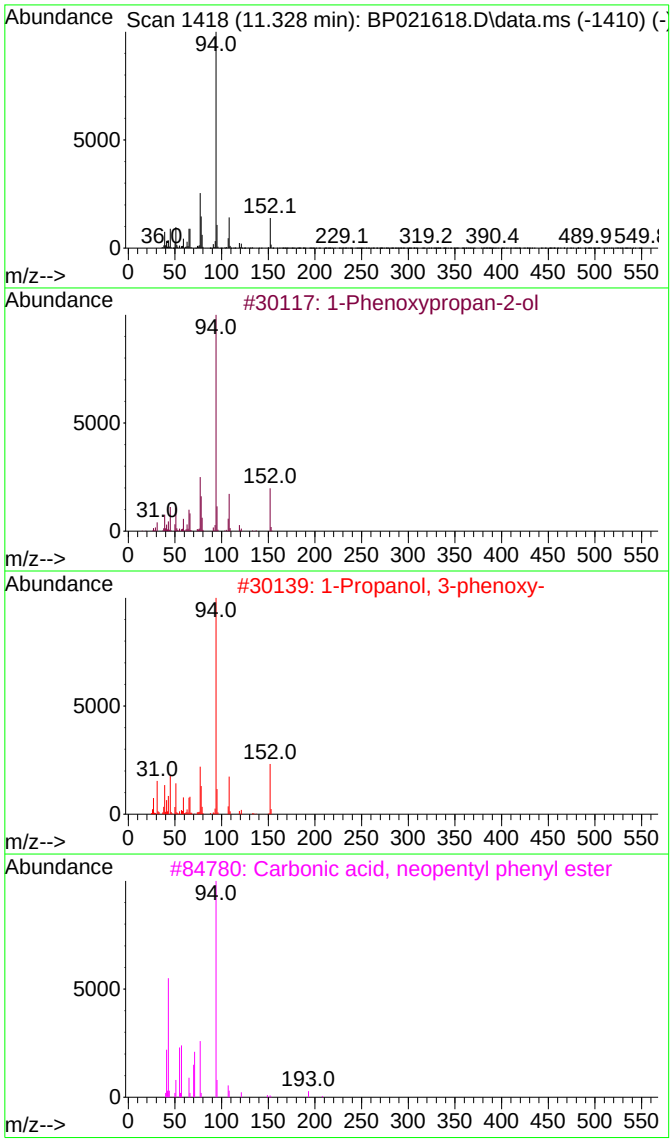
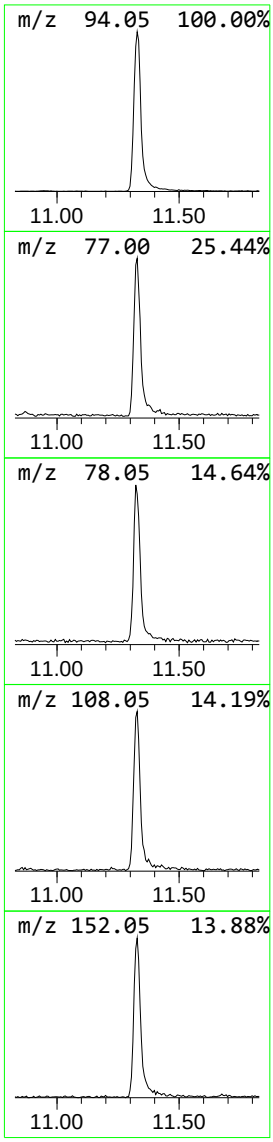
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.328	4.65 ng	654525	Naphthalene-d8	10.581

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
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TIC Library : C:\Database\NIST20.L
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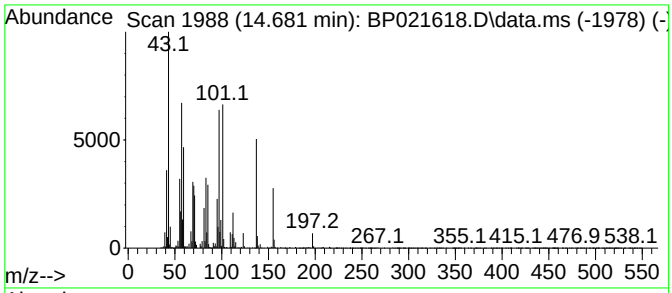
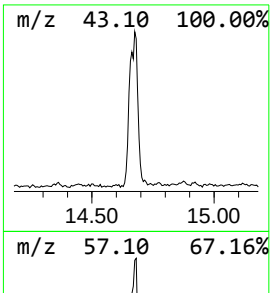
****

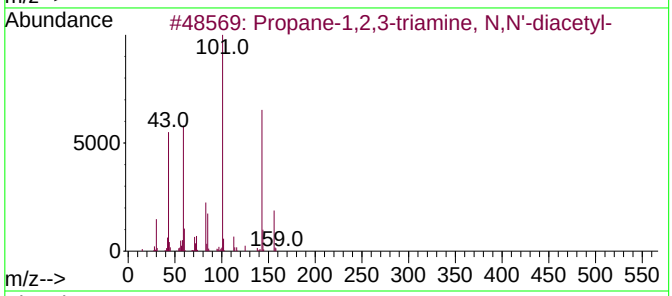
Peak Number 5 unknown14.681 Concentration Rank 6

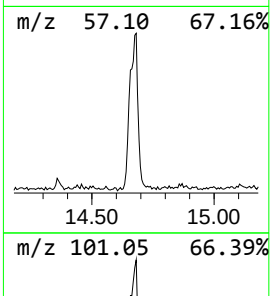
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.681	3.34 ng	622009	Acenaphthene-d10	14.445

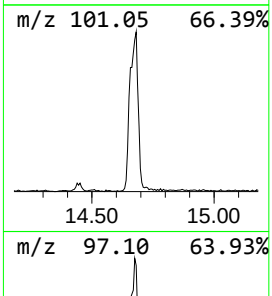
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane-1,2,3-triamine, N,N'-dia...	173	C7H15N3O2	1000500-54-4	22
2	Succinic acid, hept-2-yl 1-cyclo...	312	C18H32O4	1010391-41-2	14
3	Succinic acid, tridec-2-yn-1-yl ...	380	C23H40O4	1000390-69-6	14
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11
5	Succinic acid, hept-2-yl 4-octyl...	328	C19H36O4	1000389-56-0	10

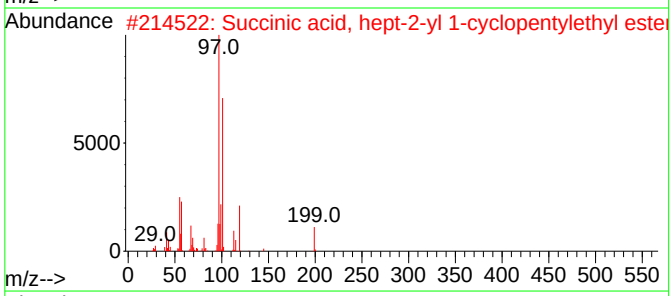


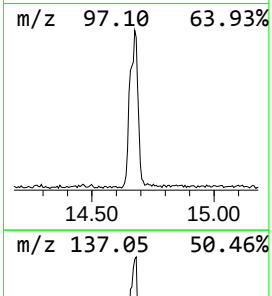


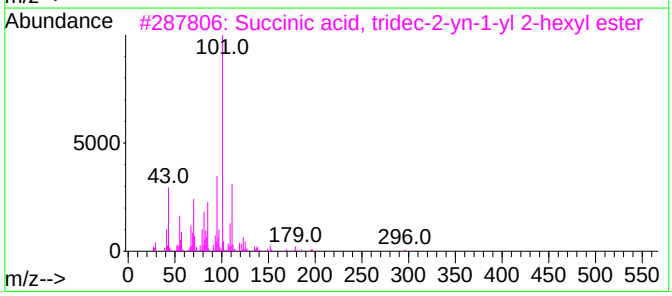


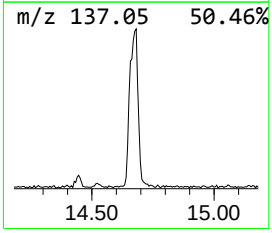












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

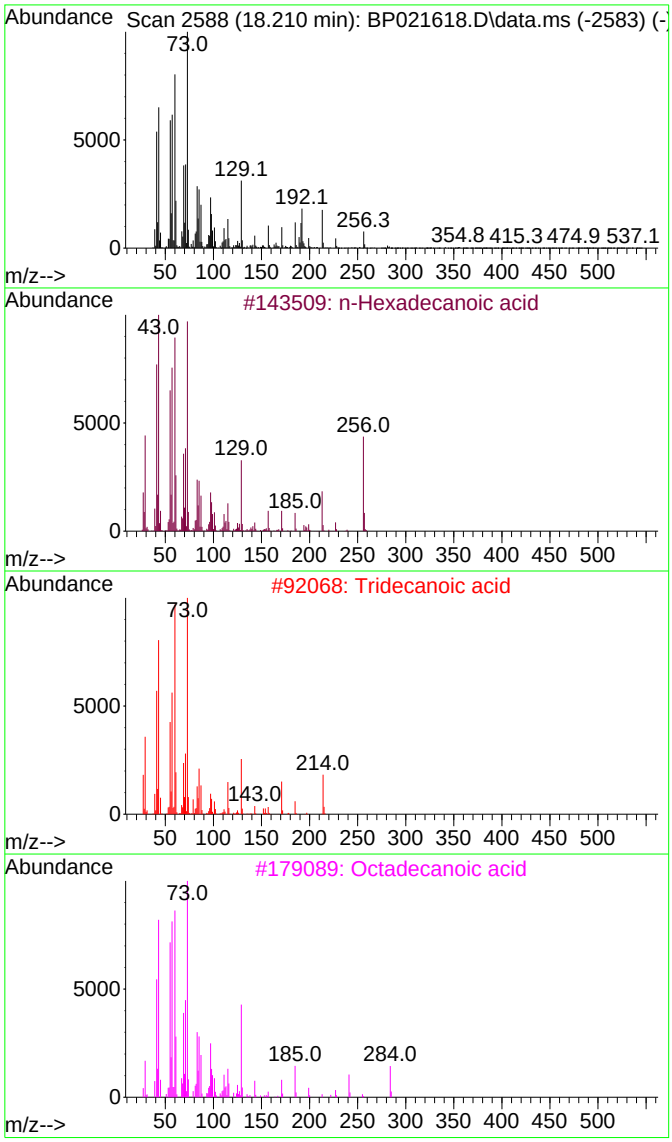
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

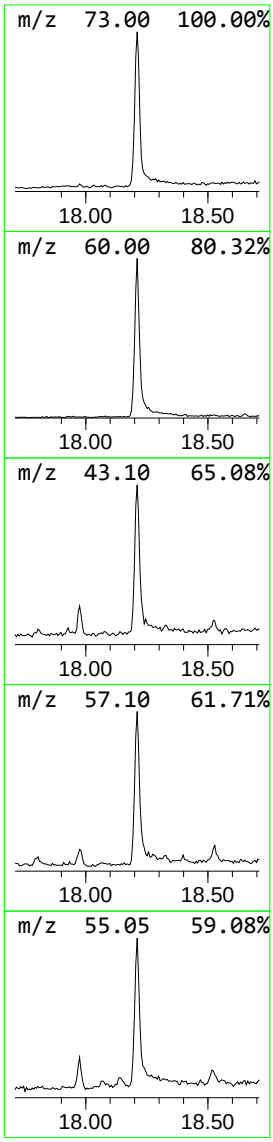
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.210	3.60 ng	814070	Phenanthrene-d10	17.257

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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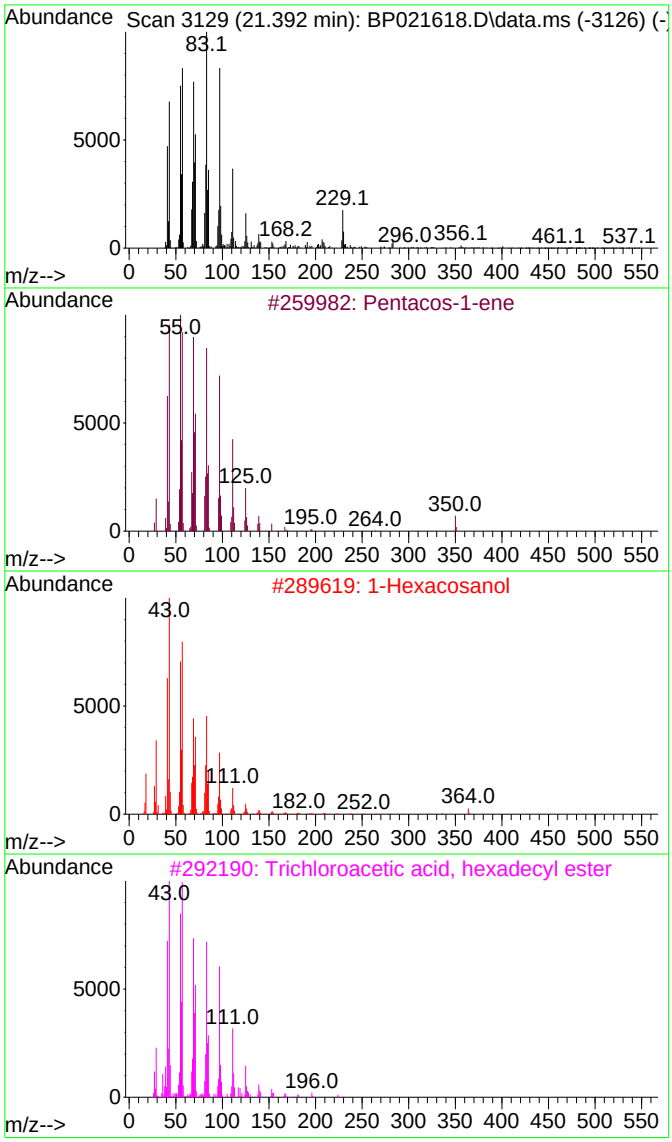
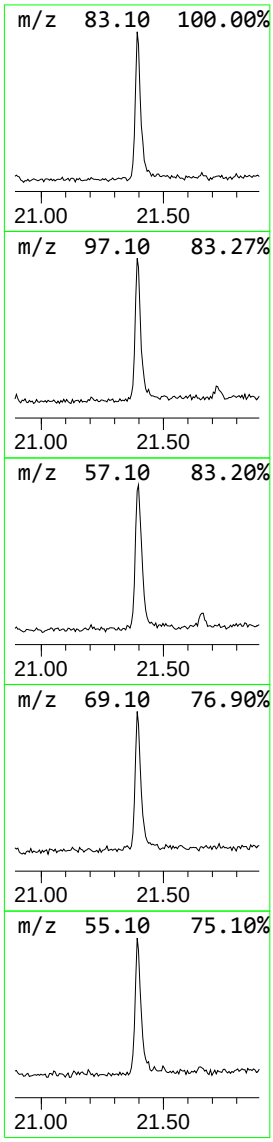
Peak Number 7 Pentacos-1-ene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.392	2.26 ng	635629	Chrysene-d12	21.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacos-1-ene	350	C25H50	016980-85-1	91
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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Operator : RC/JU
Sample : P3518-21
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OU4-TS-11-080724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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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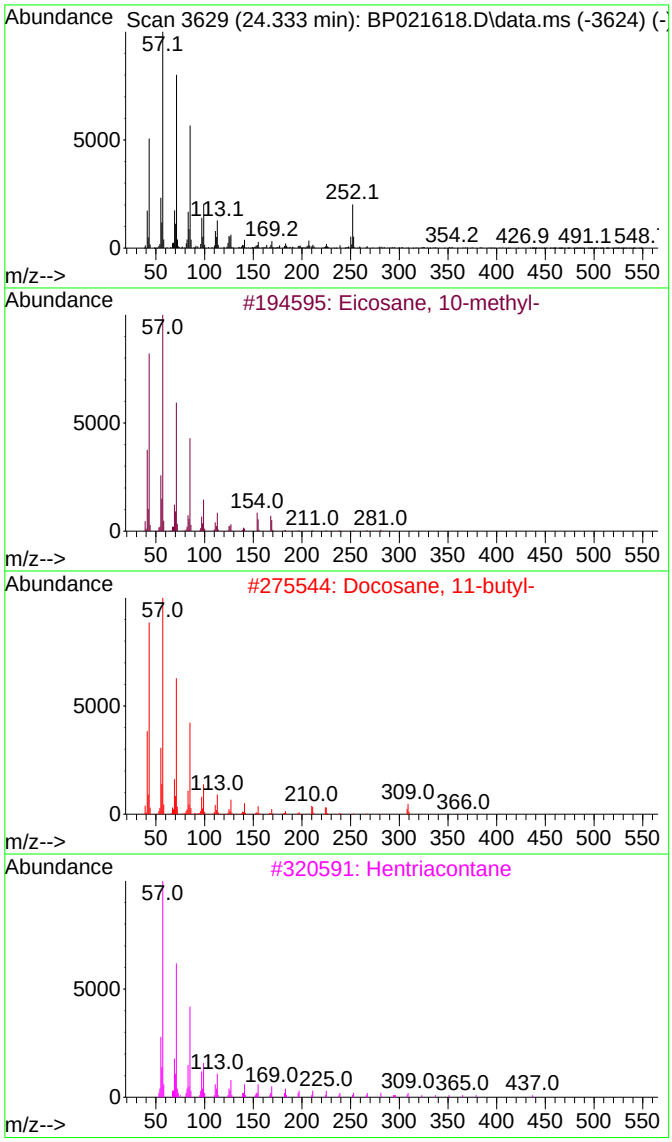
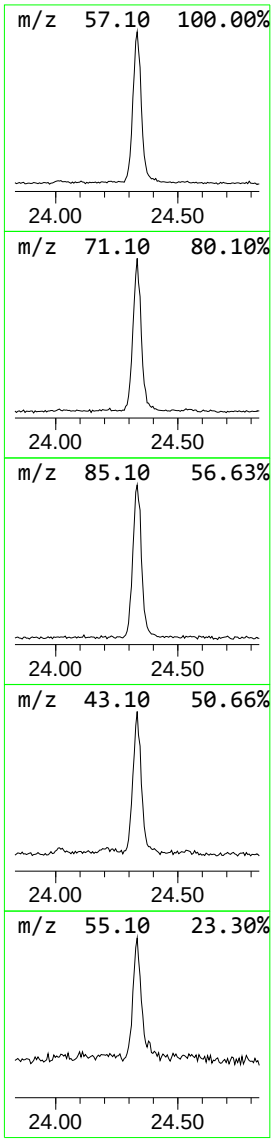
Peak Number 8 Eicosane, 10-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.333	4.47 ng	1139300	Perylene-d12	25.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	87
3	Hentriacontane	437	C31H64	000630-04-6	83
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	83
5	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP082224\
Data File : BP021618.D
Acq On : 22 Aug 2024 17:58
Operator : RC/JU
Sample : P3518-21
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
OU4-TS-11-080724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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...	3.028	32.5	ng	3221550	1	7.799	1981300	20.0
R-(-)-1,2-propa...	3.546	3.7	ng	365570	1	7.799	1981300	20.0
2-Pentanone, 4-...	4.940	3.2	ng	318403	1	7.799	1981300	20.0
1-Phenoxypropan...	11.328	4.7	ng	654525	2	10.581	2816700	20.0
unknown14.681	14.681	3.3	ng	622009	3	14.445	3722800	20.0
n-Hexadecanoic ...	18.210	3.6	ng	814070	4	17.257	4522600	20.0
Pentacos-1-ene	21.392	2.3	ng	635629	5	21.722	5625190	20.0
Eicosane, 10-me...	24.333	4.5	ng	1139300	6	25.151	5093000	20.0