LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
Data File : BF140721.D
Acq On : 03 Dec 2024 19:44
Operator : RC/JU
Sample : P5052-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-62

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_F\Methods\8270-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140721.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	22	rVB	667860	1082864	60.43%	8.623%
2	2.252	22	27	34	rVB	28151	46392	2.59%	0.369%
3	5.093	504	510	526	rVB	96958	159218	8.88%	1.268%
4	5.504	574	580	594	rBV	1105514	1481832	82.69%	11.800%
5	6.510	745	751	773	rBV	1132651	1534731	85.64%	12.221%
6	6.869	807	812	818	rVB	321066	388241	21.66%	3.092%
7	7.434	902	908	917	rBV	746043	987484	55.10%	7.864%
8	7.686	945	951	960	rBV	25221	42964	2.40%	0.342%
9	8.151	1022	1030	1042	rBV	354963	484311	27.03%	3.857%
10	9.222	1207	1212	1222	rBV	1437366	1792021	100.00%	14.270%
11	9.904	1323	1328	1340	rVB	398318	503766	28.11%	4.012%
12	10.616	1444	1449	1458	rBV	157374	200700	11.20%	1.598%
13	10.698	1458	1463	1475	rBV	677863	900882	50.27%	7.174%
14	11.398	1576	1582	1590	rBV	319414	440224	24.57%	3.506%
15	11.916	1664	1670	1683	rBV3	60025	123627	6.90%	0.984%
16	12.010	1683	1686	1694	rVB4	8322	18180	1.01%	0.145%
17	12.645	1791	1794	1799	rVB2	20575	27361	1.53%	0.218%
18	12.845	1823	1828	1834	rBV	22135	41541	2.32%	0.331%
19	12.980	1846	1851	1859	rVB	994418	1253026	69.92%	9.978%
20	13.874	1998	2003	2011	rBV	71452	136883	7.64%	1.090%
21	14.051	2028	2033	2040	rBV	277232	378541	21.12%	3.014%
22	14.815	2160	2163	2168	rBV2	40875	58456	3.26%	0.466%
23	15.557	2284	2289	2298	rVB	212065	325577	18.17%	2.593%
24	16.698	2479	2483	2490	rVB	77696	148855	8.31%	1.185%

Sum of corrected areas: 12557677

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120324\
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Misc :
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Instrument :
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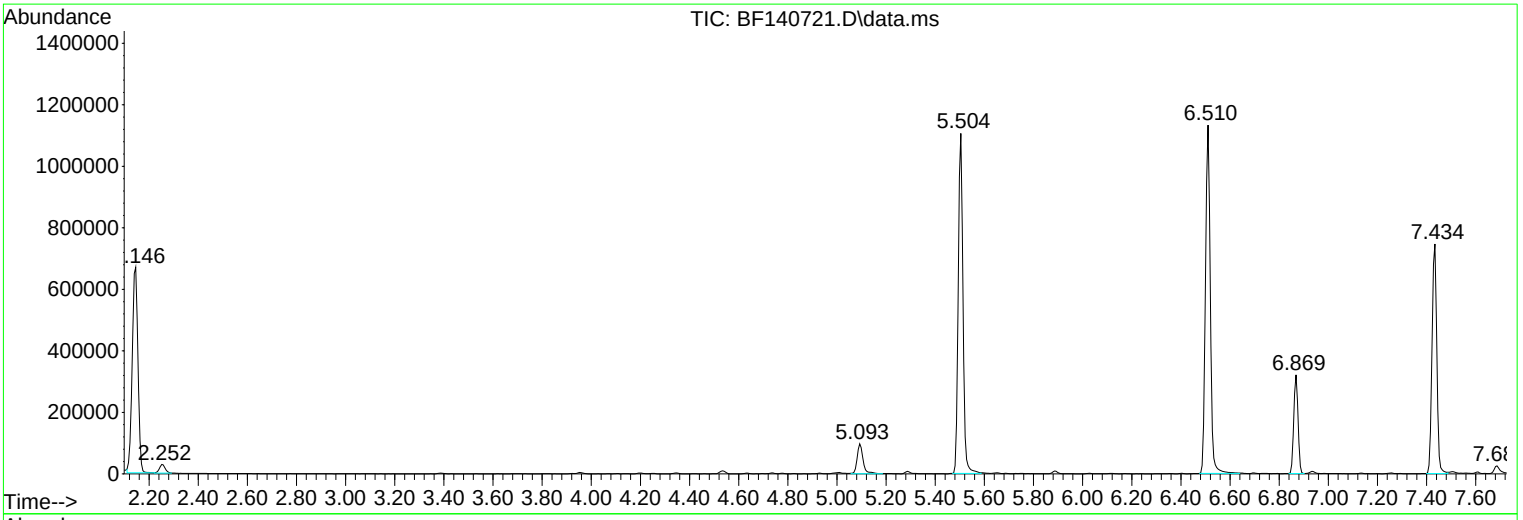
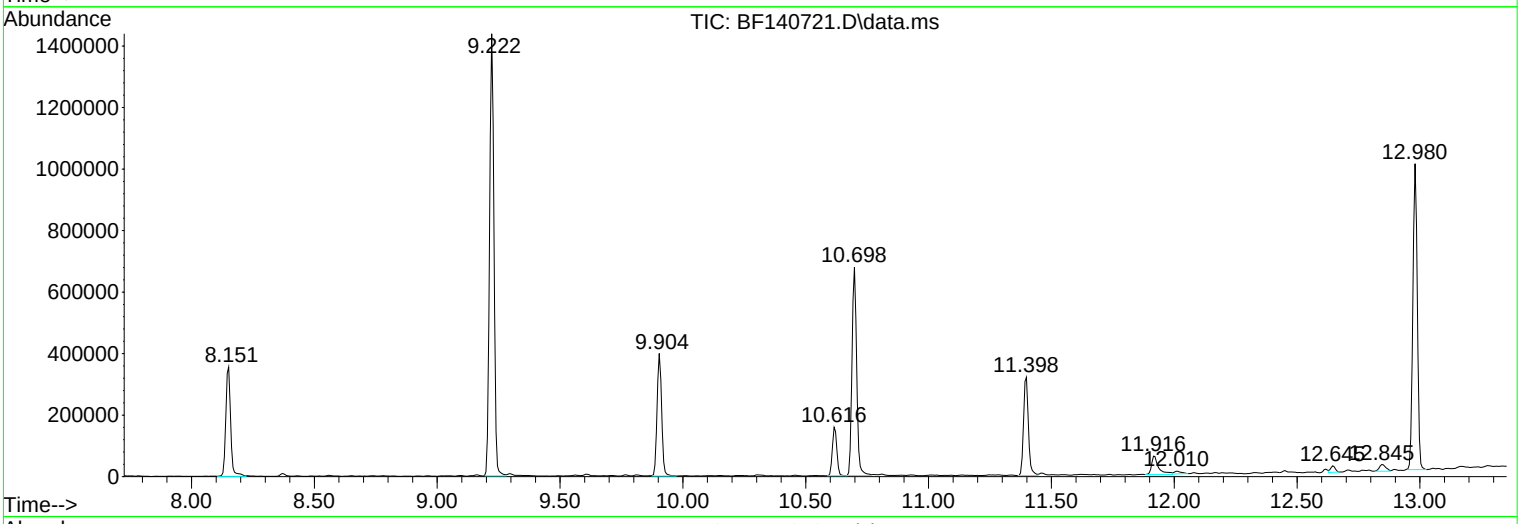
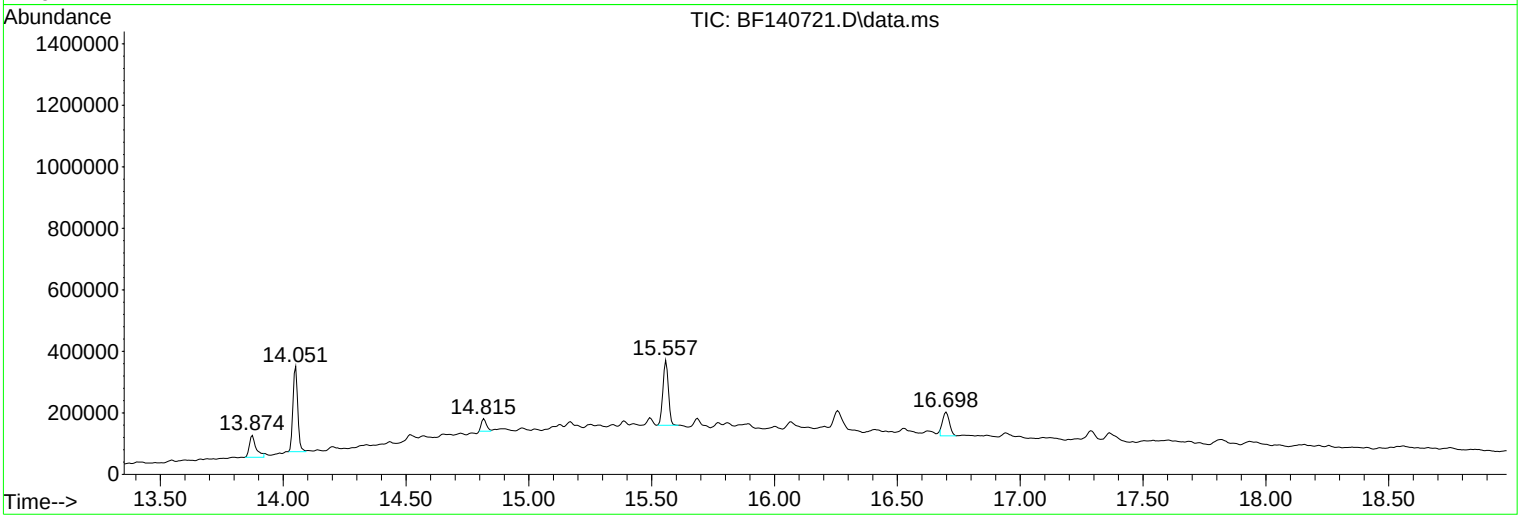
ClientSampleId :
OR-640-COMP-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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

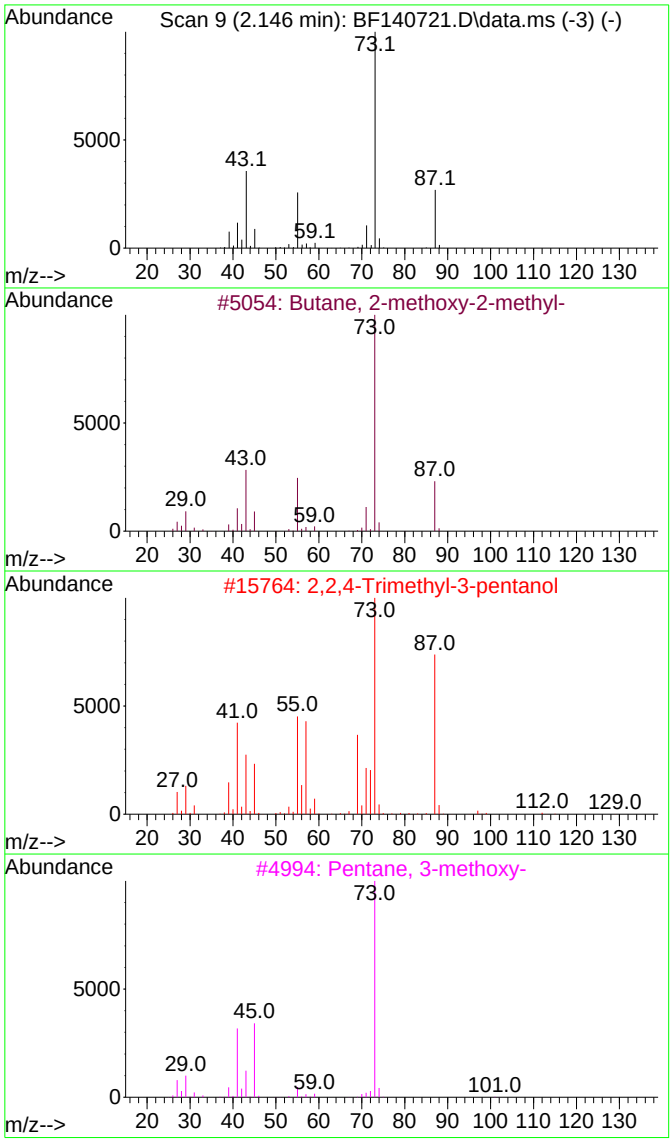
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

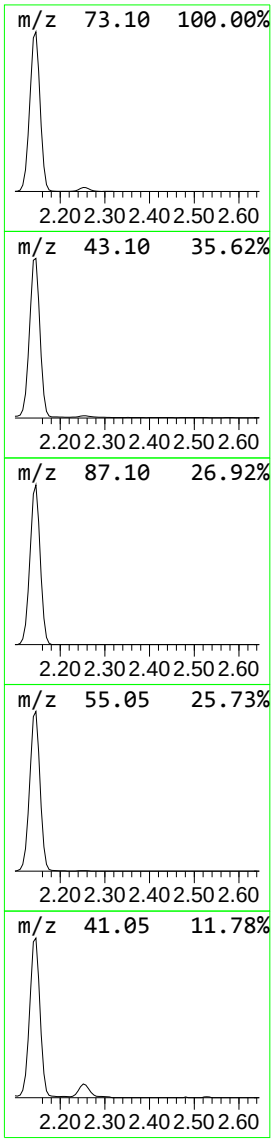
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	55.78 ng	1082860	1,4-Dichlorobenzene-d4	6.869

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Acq On : 03 Dec 2024 19:44
Operator : RC/JU
Sample : P5052-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OR-640-COMP-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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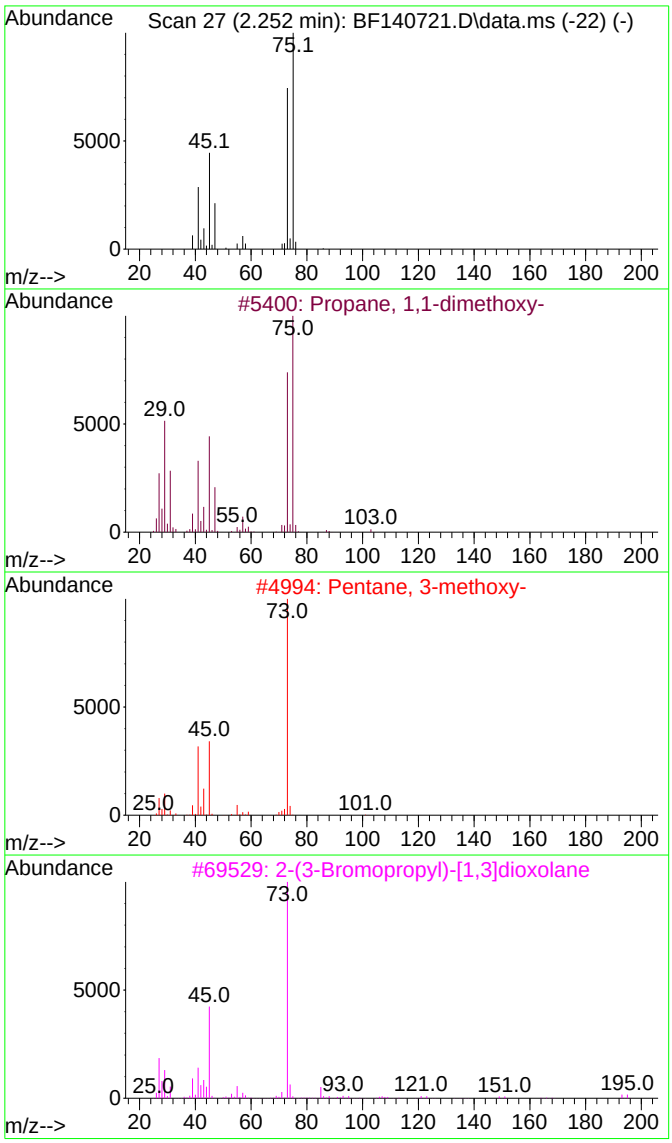
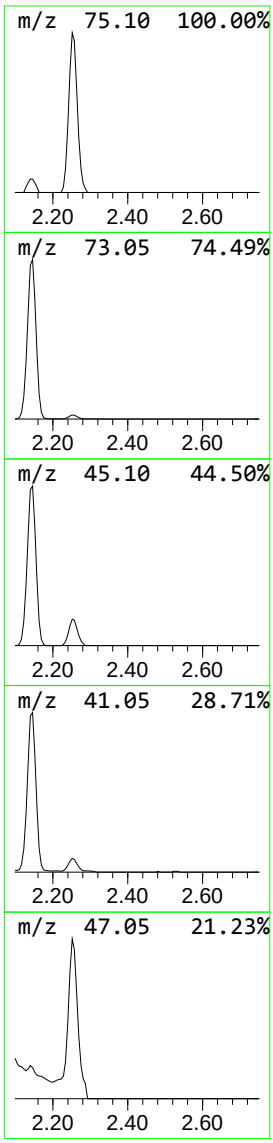
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	2.39 ng	46392	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3	2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	9
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9





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Sample : P5052-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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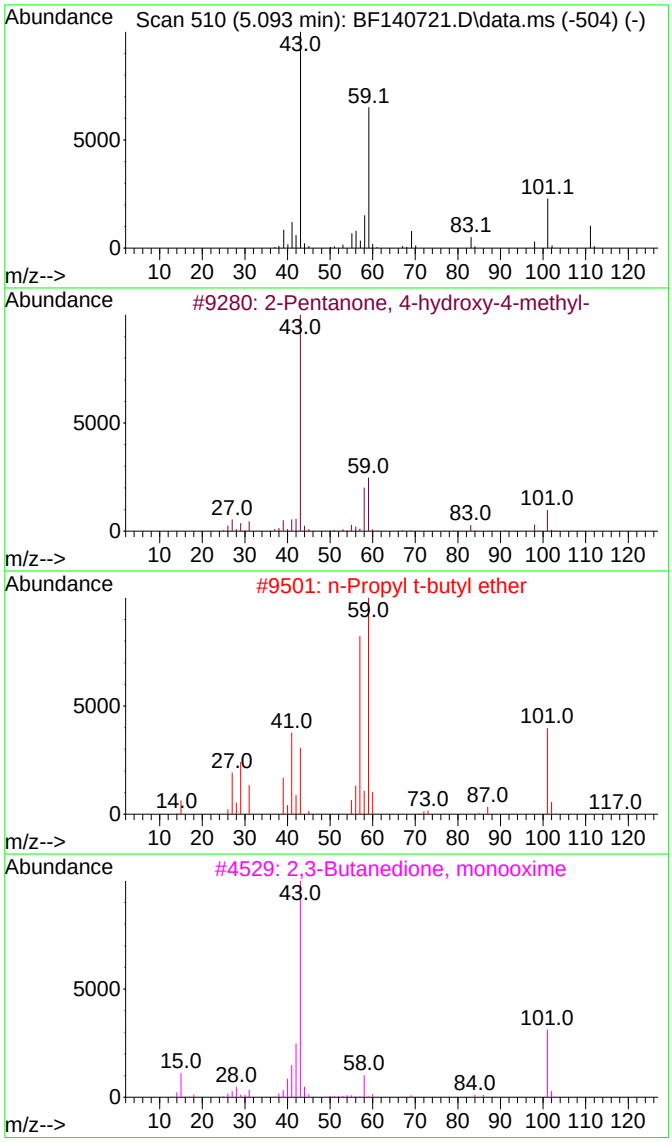
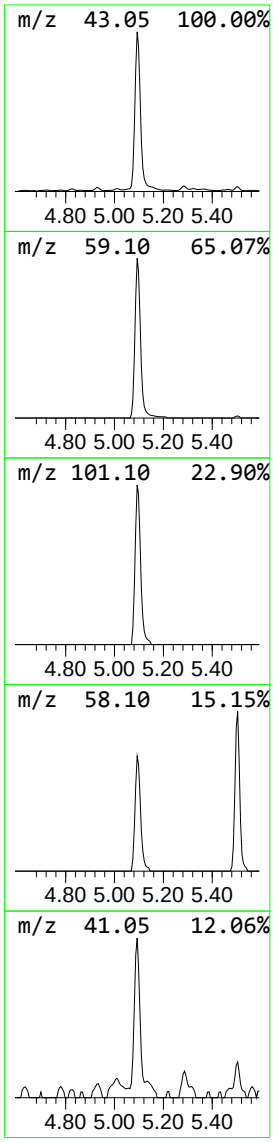
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	8.20 ng	159218	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	17
5	Hexane, 1-ethoxy-	130	C8H18O	005756-43-4	12





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Operator : RC/JU
Sample : P5052-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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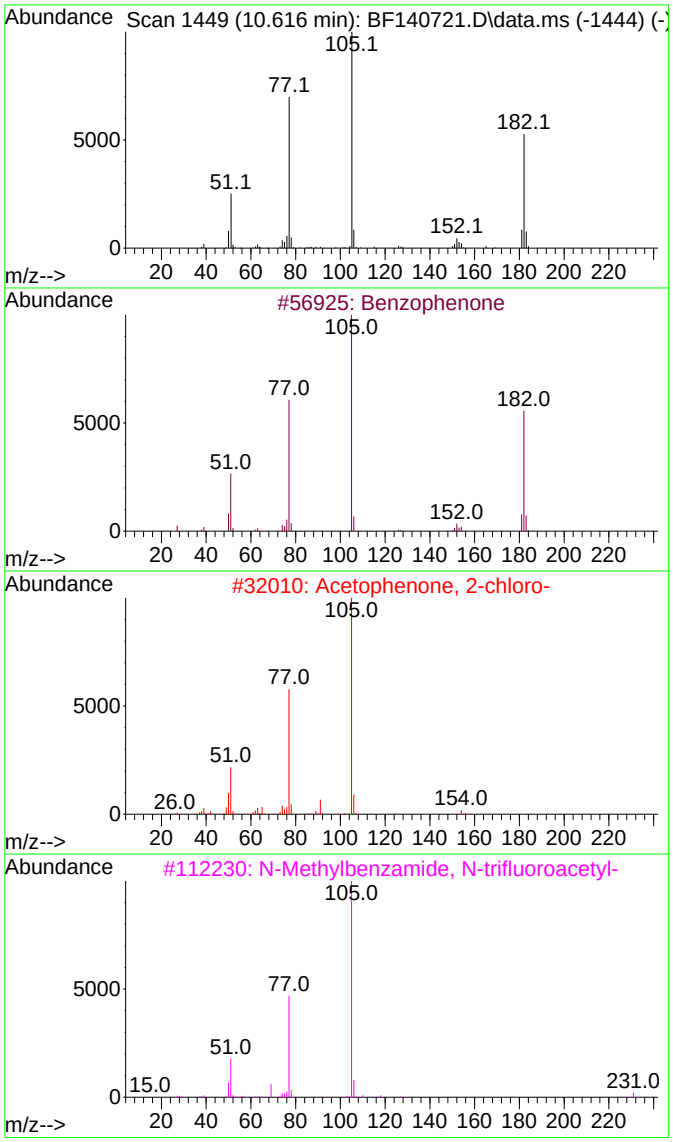
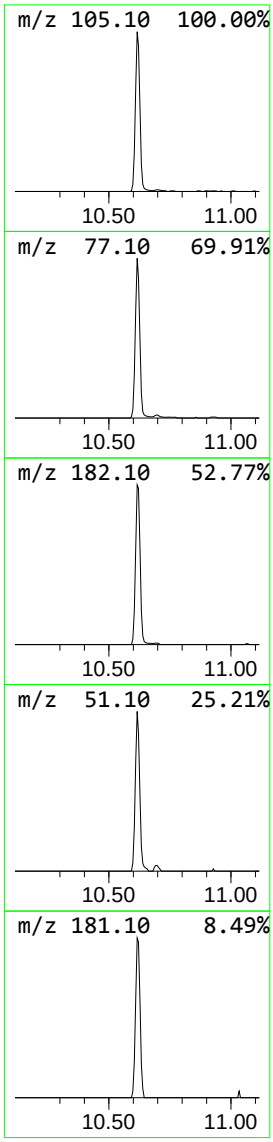
Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	7.97 ng	200700	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47





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Operator : RC/JU
Sample : P5052-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-640-COMP-62

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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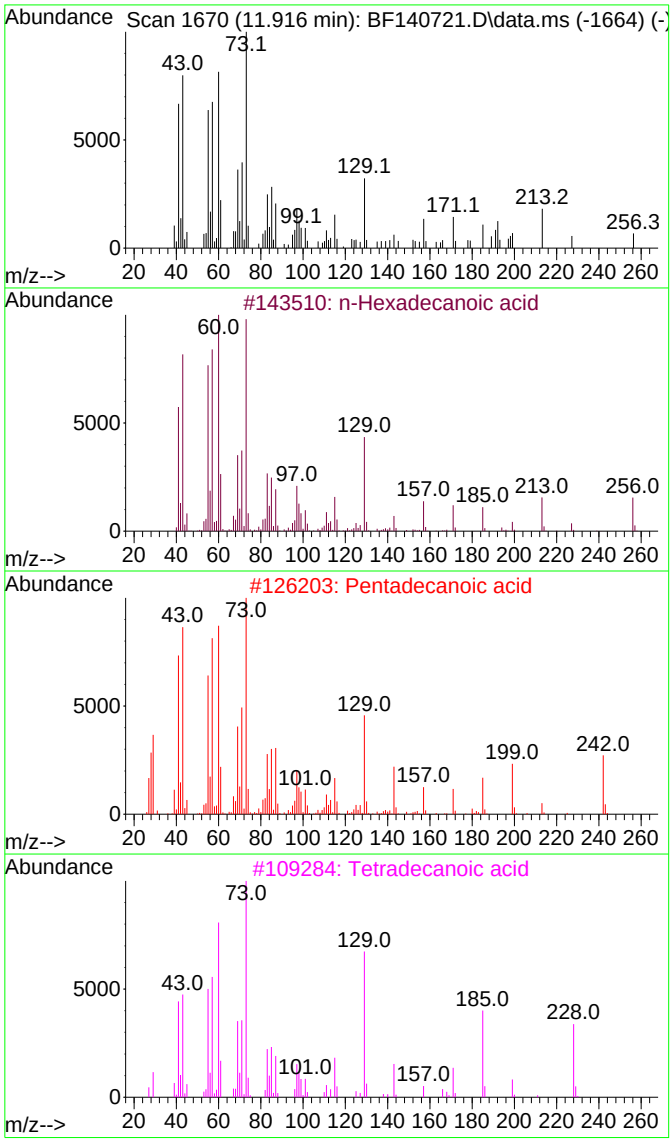
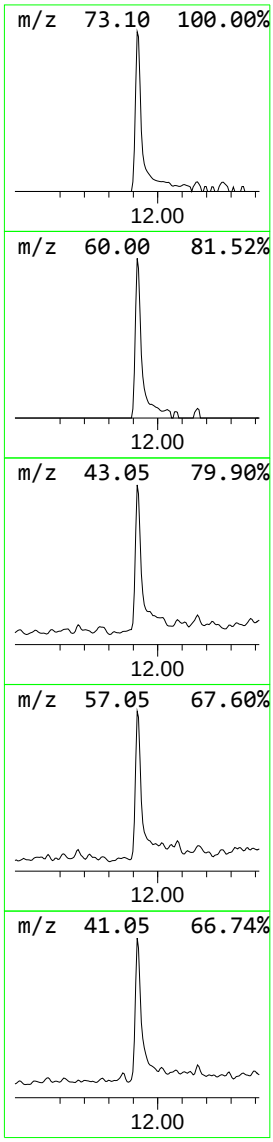
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	5.62 ng	123627	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tetradecane	198	C14H30	000629-59-4	56
5	Nonanoic acid	158	C9H18O2	000112-05-0	46





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
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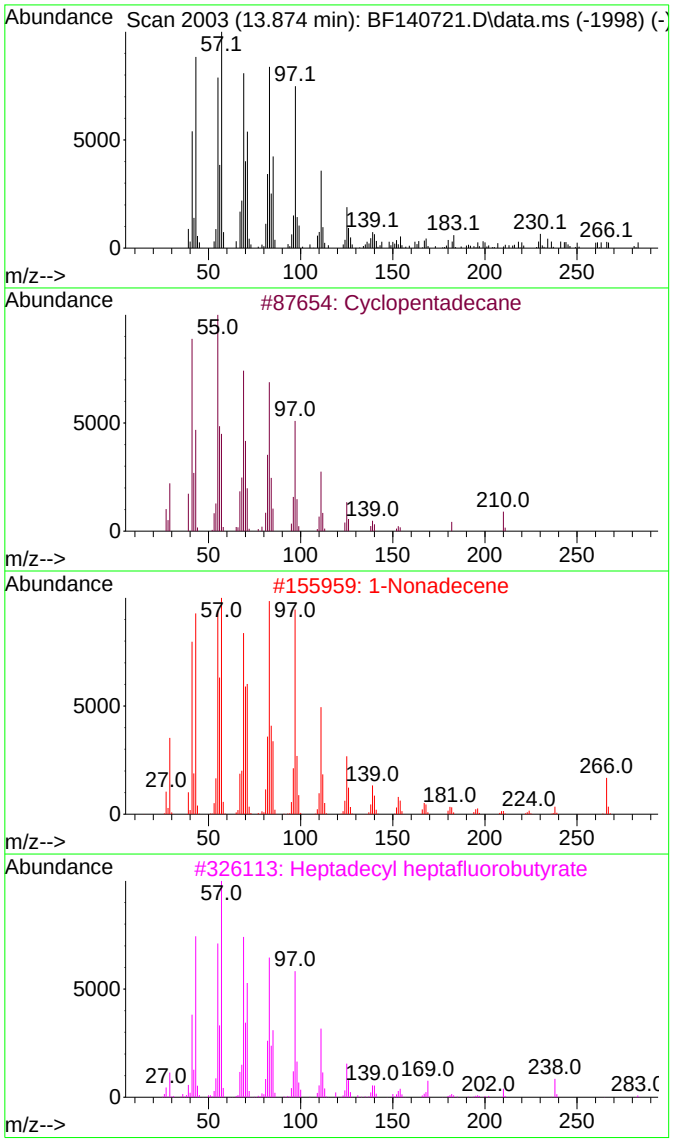
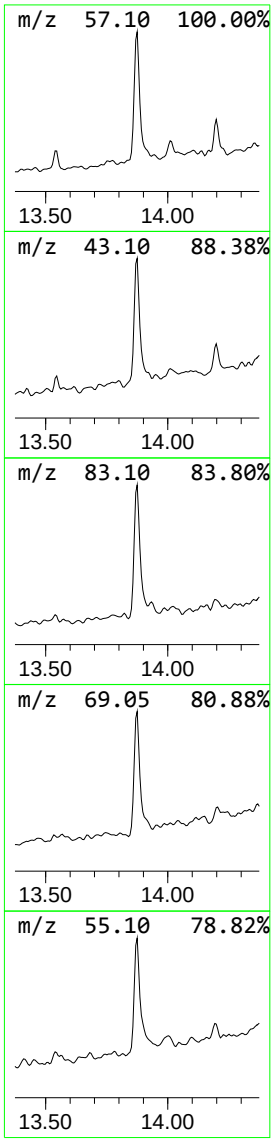
Peak Number 7 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	7.23 ng	136883	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	1-Nonadecene	266	C19H38	018435-45-5	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	93





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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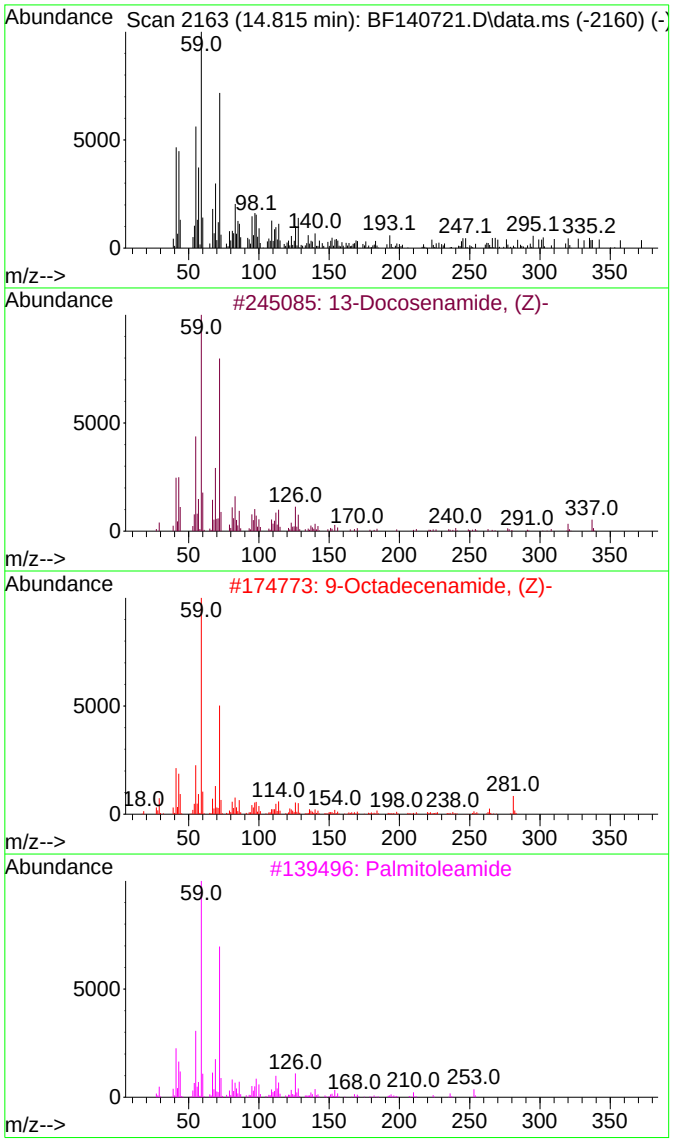
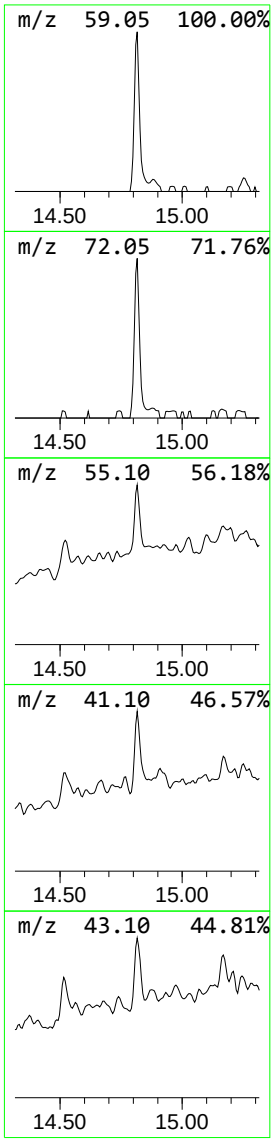
Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	3.59 ng	58456	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	89
3	Palmitoleamide	253	C16H31NO	106010-22-4	64
4	Hexadecanamide	255	C16H33NO	000629-54-9	50
5	Nonanamide	157	C9H19NO	001120-07-6	47





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TIC Library : C:\Database\NIST20.L
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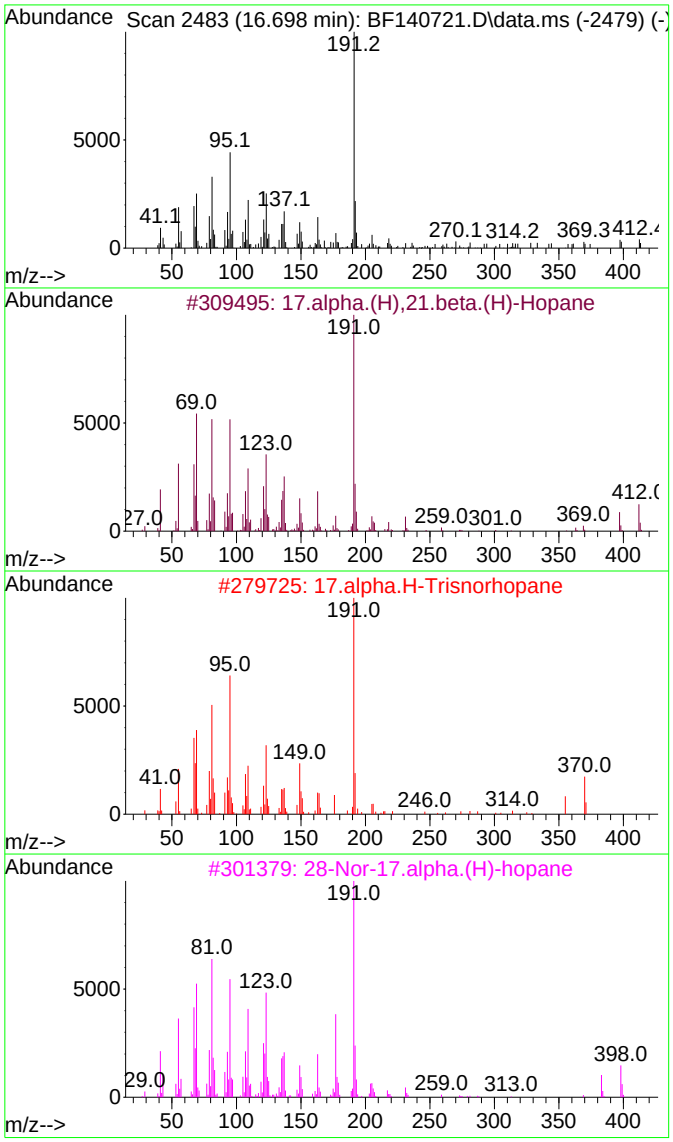
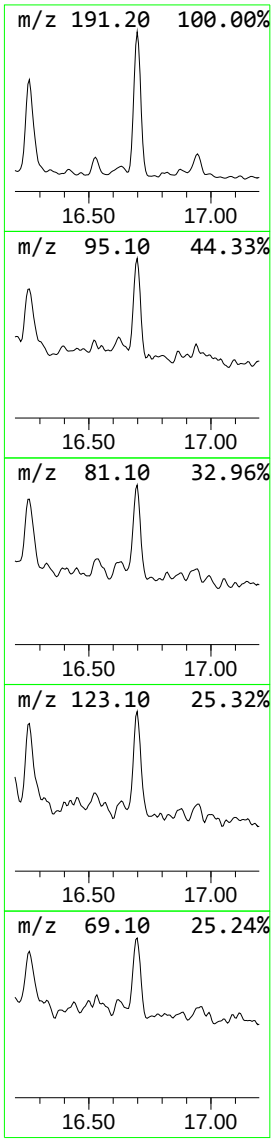
Peak Number 9 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.698	9.14 ng	148855	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	93
2	17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	93
3	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	49
4	Benzoic acid, 4-[3-(3,4-dimethox...	397	C23H27NO5	1010317-25-8	38
5	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	38





Tentatively Identified Compound (LSC) summary

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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...	2.146	55.8	ng	1082860	1	6.869	388241	20.0
Propane, 1,1-di...	2.252	2.4	ng	46392	1	6.869	388241	20.0
2-Pentanone, 4-...	5.093	8.2	ng	159218	1	6.869	388241	20.0
Benzophenone	10.616	8.0	ng	200700	3	9.904	503766	20.0
n-Hexadecanoic ...	11.916	5.6	ng	123627	4	11.398	440224	20.0
Cyclopentadecane	13.874	7.2	ng	136883	5	14.051	378541	20.0
13-Docosenamide...	14.815	3.6	ng	58456	6	15.557	325577	20.0
17.alpha.(H),21...	16.698	9.1	ng	148855	6	15.557	325577	20.0