LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138841.D
Acq On : 07 Aug 2024 14:34
Operator : RC/JU
Sample : P3450-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

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-BF073024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138841.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	8	14	rVB	1483612	2263900	100.00%	22.516%
2	5.057	499	504	513	rVB	25878	36062	1.59%	0.359%
3	5.469	569	574	599	rBB	428196	567152	25.05%	5.641%
4	5.716	612	616	623	rBV	24601	30740	1.36%	0.306%
5	6.481	741	746	758	rBV	252691	347579	15.35%	3.457%
6	6.839	802	807	812	rBV	208915	257328	11.37%	2.559%
7	7.404	897	903	908	rBV	695680	942504	41.63%	9.374%
8	8.116	1019	1024	1030	rBV	265608	346309	15.30%	3.444%
9	8.433	1070	1078	1093	rBV	39420	63083	2.79%	0.627%
10	9.192	1201	1207	1212	rBV	1331183	1712254	75.63%	17.030%
11	9.869	1317	1322	1332	rVB	310109	389709	17.21%	3.876%
12	10.663	1451	1457	1466	rBV	702951	912994	40.33%	9.080%
13	11.357	1570	1575	1586	rBV	294152	364152	16.09%	3.622%
14	11.880	1659	1664	1675	rBV3	22620	43764	1.93%	0.435%
15	12.939	1838	1844	1849	rBV	1002304	1267287	55.98%	12.604%
16	13.468	1928	1934	1940	rBV	23592	34058	1.50%	0.339%
17	13.845	1992	1998	2011	rBV3	17293	44095	1.95%	0.439%
18	13.992	2018	2023	2031	rVB	151864	200992	8.88%	1.999%
19	15.457	2266	2272	2281	rVB	133595	202840	8.96%	2.017%
20	16.339	2415	2422	2434	rBV9	7858	27679	1.22%	0.275%

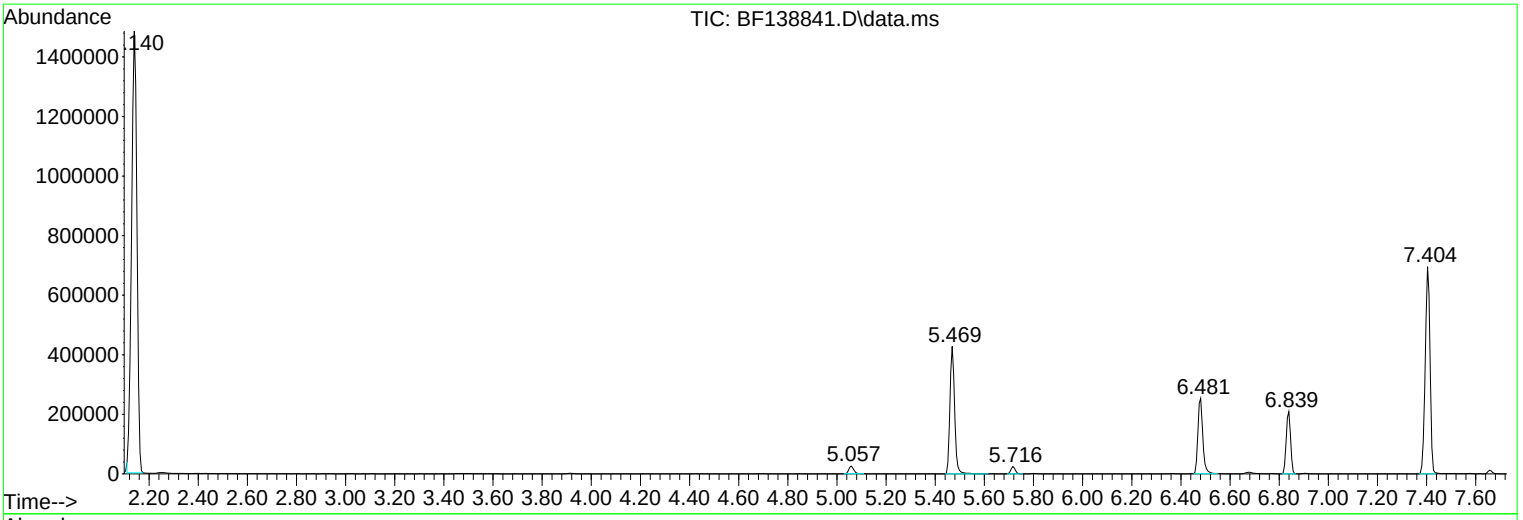
Sum of corrected areas: 10054481

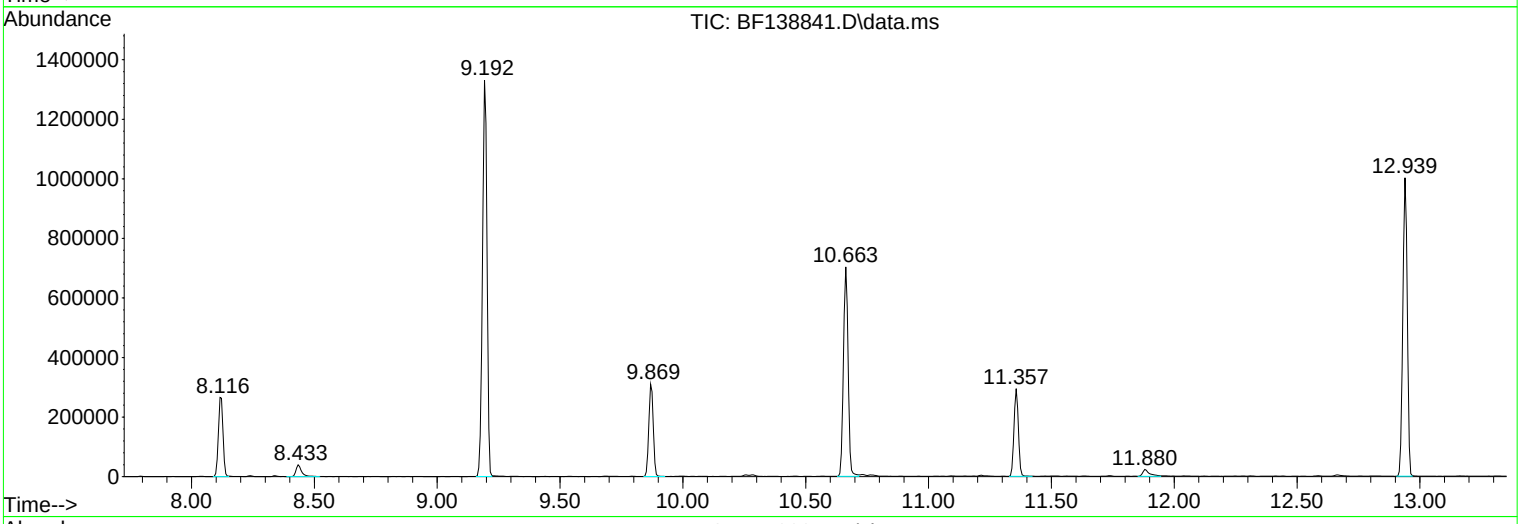
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138841.D
Acq On : 07 Aug 2024 14:34
Operator : RC/JU
Sample : P3450-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

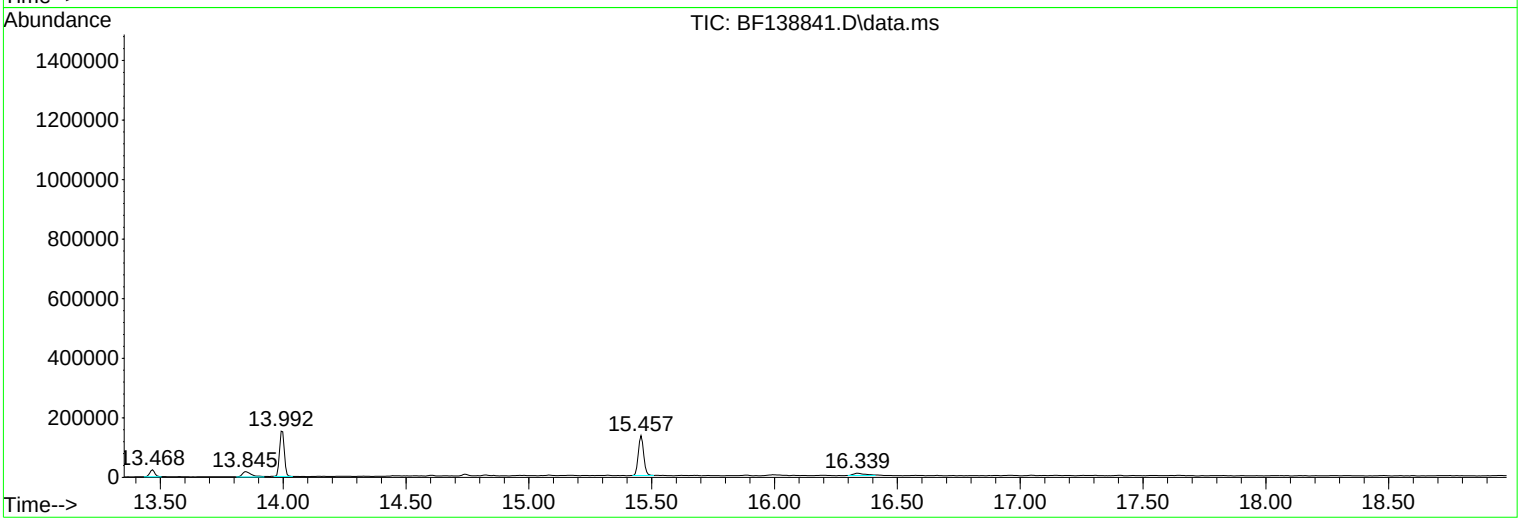
Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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_F\Data\BF080724\
Data File : BF138841.D
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Operator : RC/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

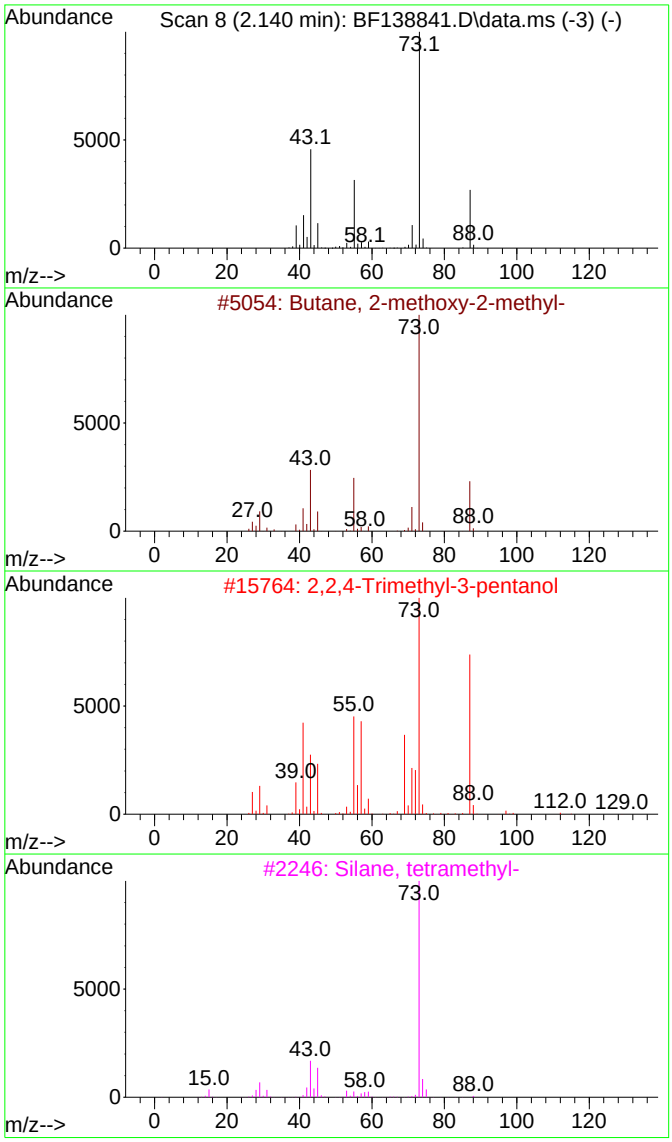
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

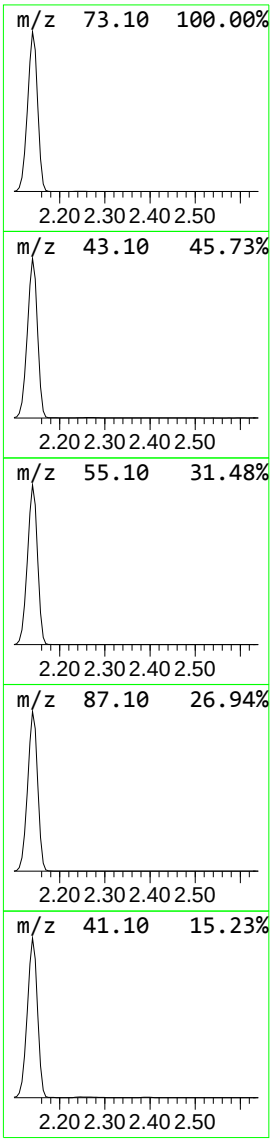
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	175.95 ng	2263900	1,4-Dichlorobenzene-d4	6.839

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	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138841.D
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Operator : RC/JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

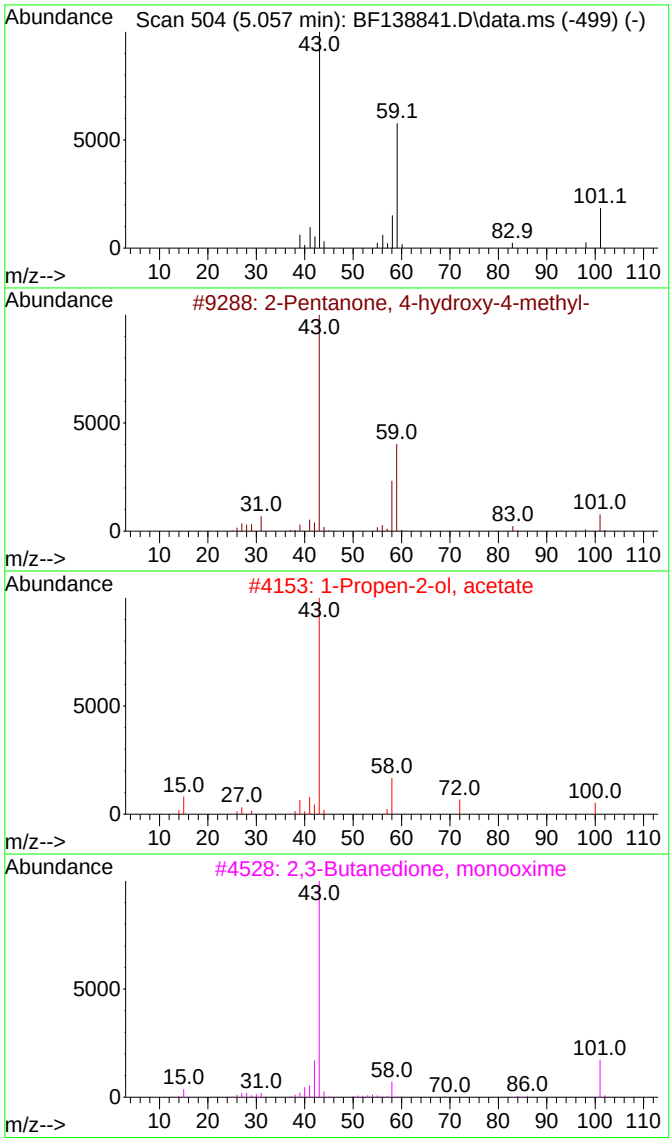
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

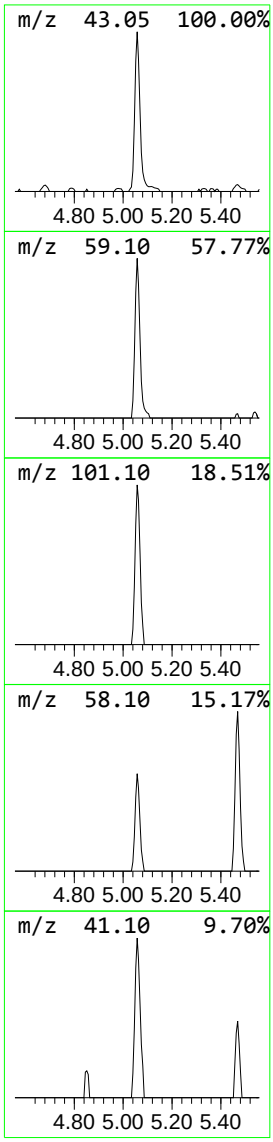
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.80 ng	36062	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
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Operator : RC/JU
Sample : P3450-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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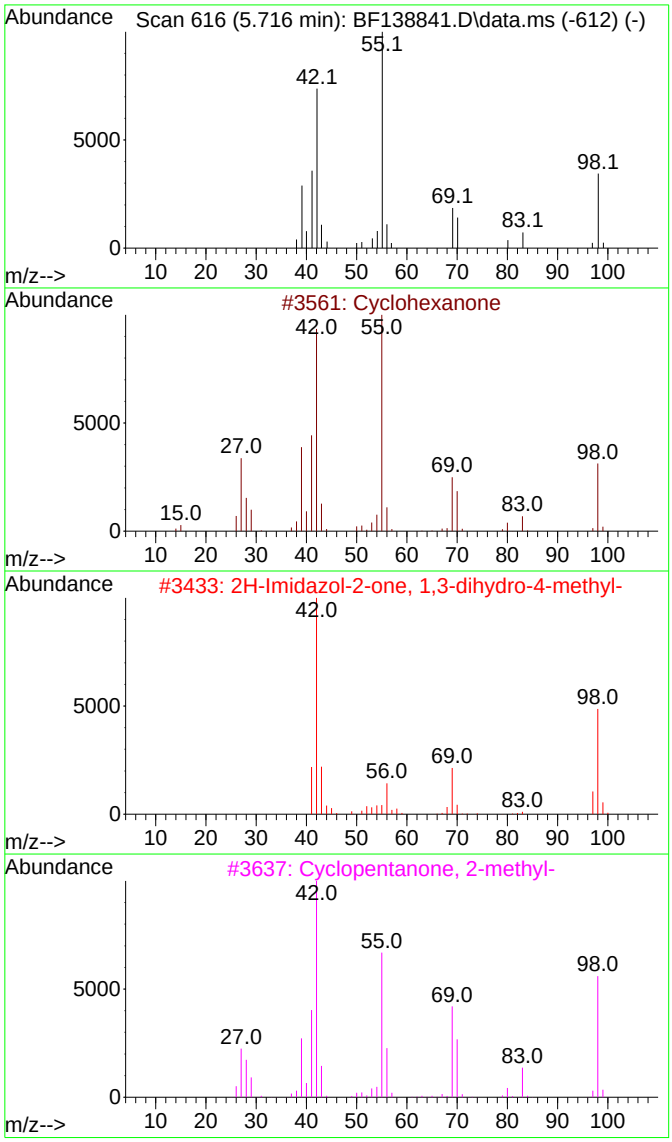
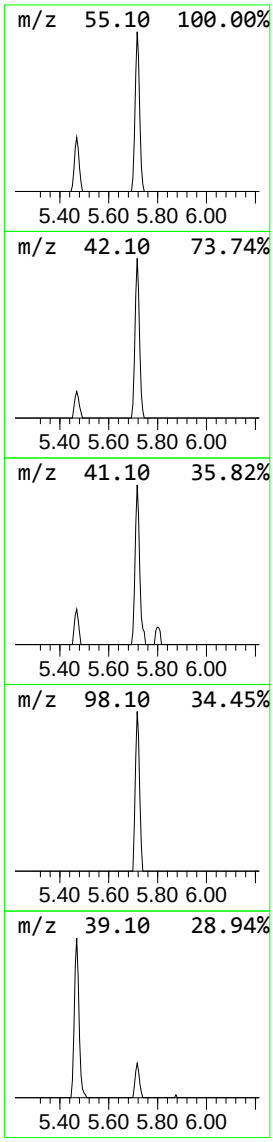
****

Peak Number 3 Cyclohexanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.716	2.39 ng	30740	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone	98	C6H10O	000108-94-1	95
2	2H-Imidazol-2-one, 1,3-dihydro-4...	98	C4H6N2O	001192-34-3	59
3	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	52
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	47
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138841.D
Acq On : 07 Aug 2024 14:34
Operator : RC/JU
Sample : P3450-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

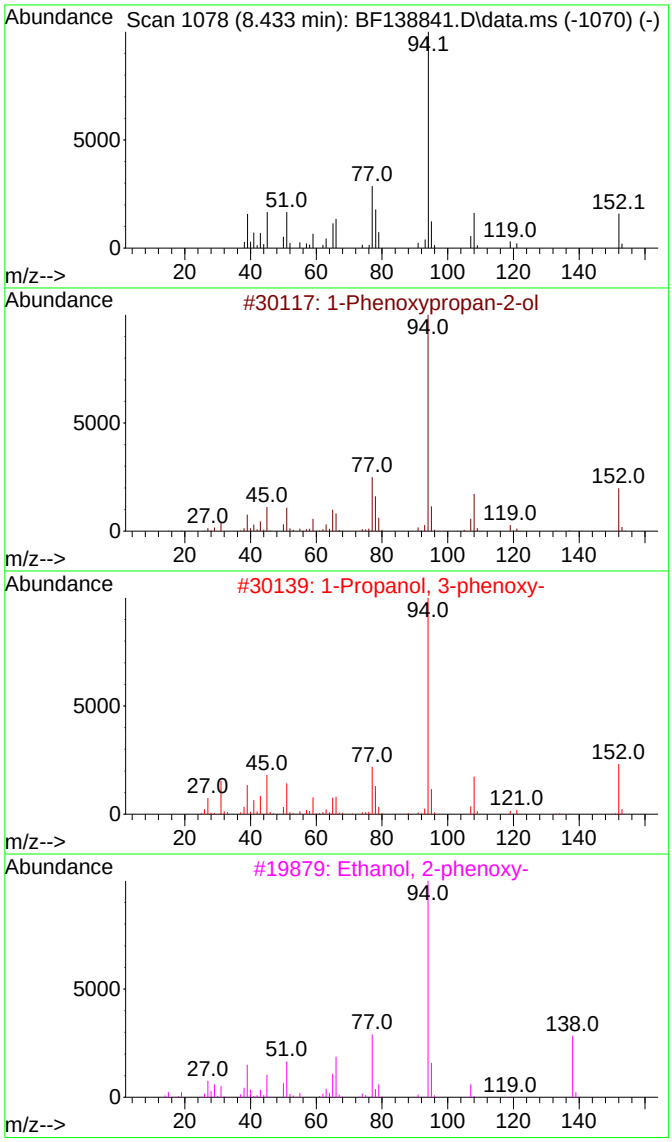
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

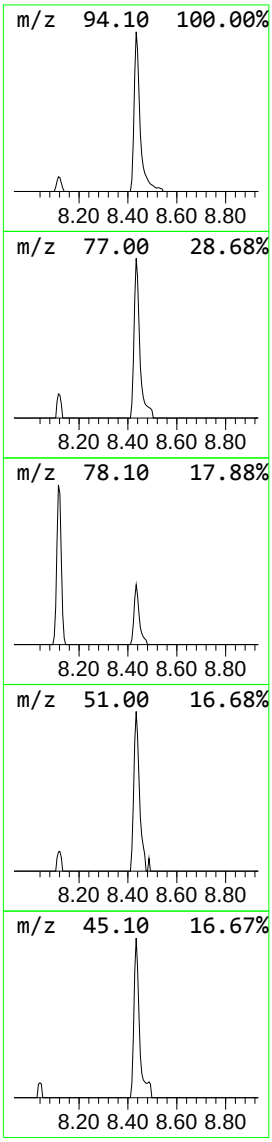
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.64 ng	63083	Naphthalene-d8	8.122

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	59
5	Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138841.D
Acq On : 07 Aug 2024 14:34
Operator : RC/JU
Sample : P3450-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

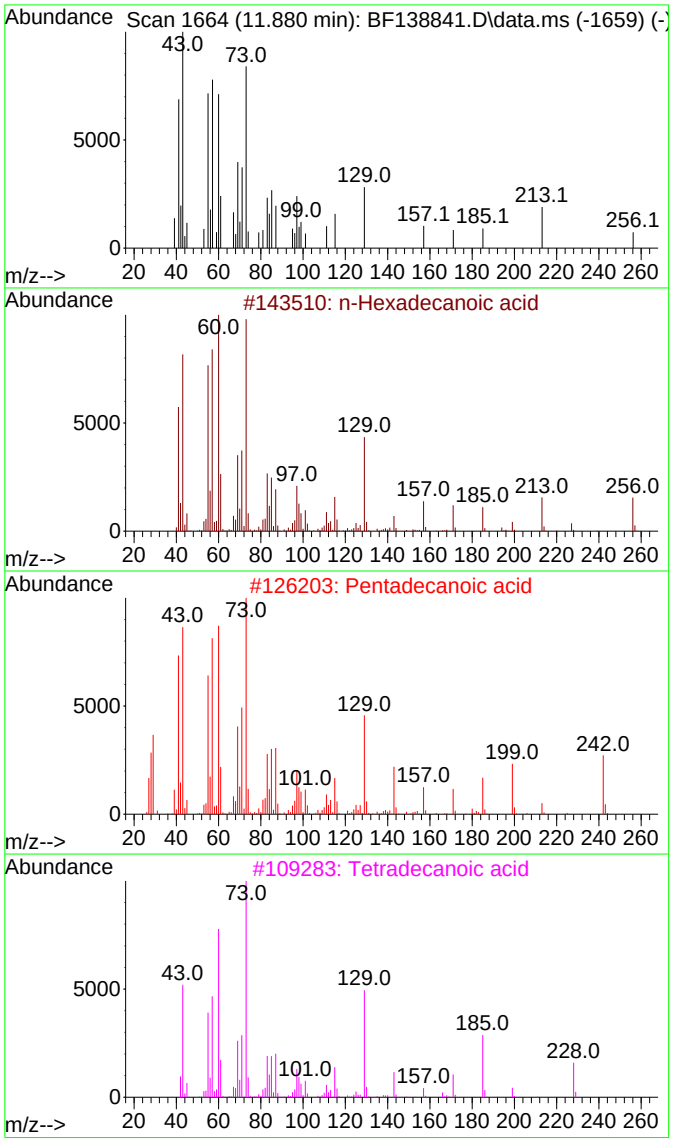
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

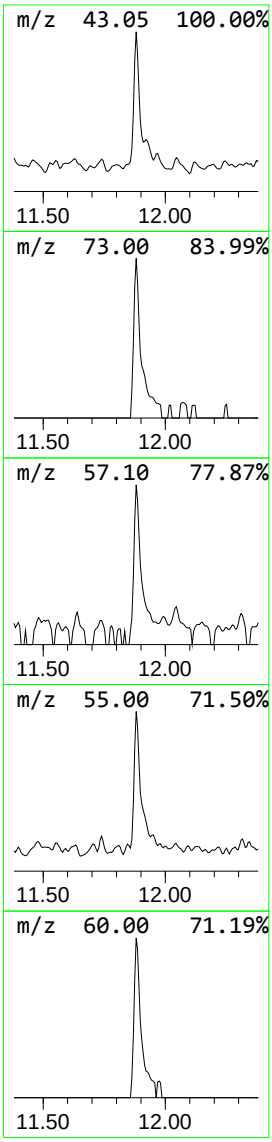
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.40 ng	43764	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138841.D
Acq On : 07 Aug 2024 14:34
Operator : RC/JU
Sample : P3450-01
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Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

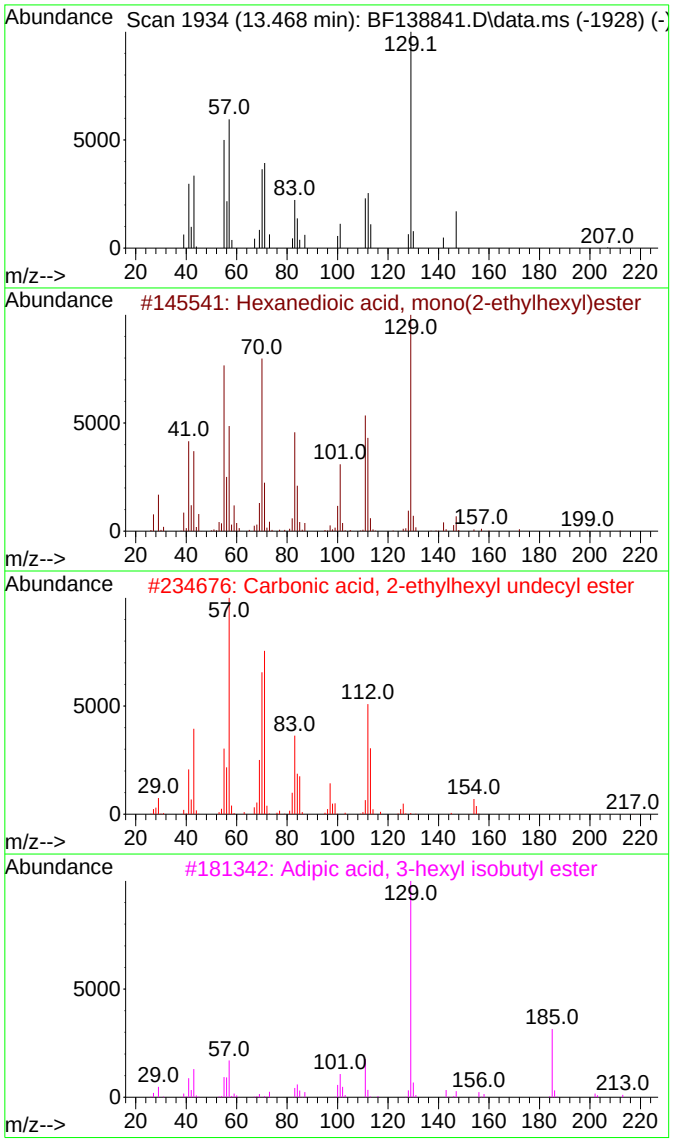
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

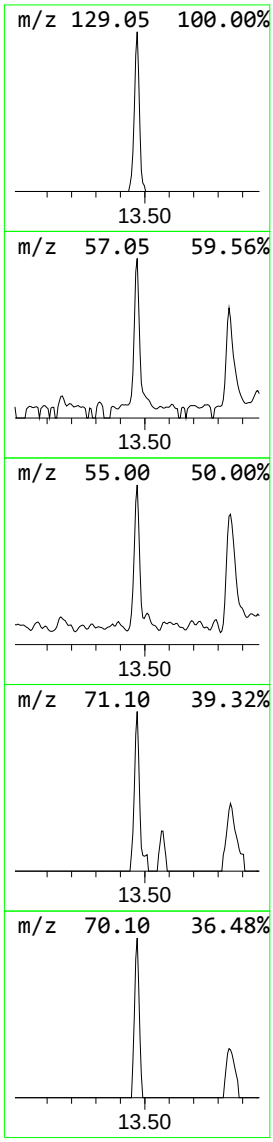
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexanedioic acid, mono(2-et... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.469	3.39 ng	34058	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	59
2	Carbonic acid, 2-ethylhexyl unde...	328	C20H40O3	1000383-13-8	38
3	Adipic acid, 3-hexyl isobutyl ester	286	C16H30O4	1000353-62-2	38
4	Dichloroacetic acid, 2-octyl ester	240	C10H18Cl2O2	096980-53-9	35
5	Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
Data File : BF138841.D
Acq On : 07 Aug 2024 14:34
Operator : RC/JU
Sample : P3450-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
921-J-WP0-0.25-080124

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

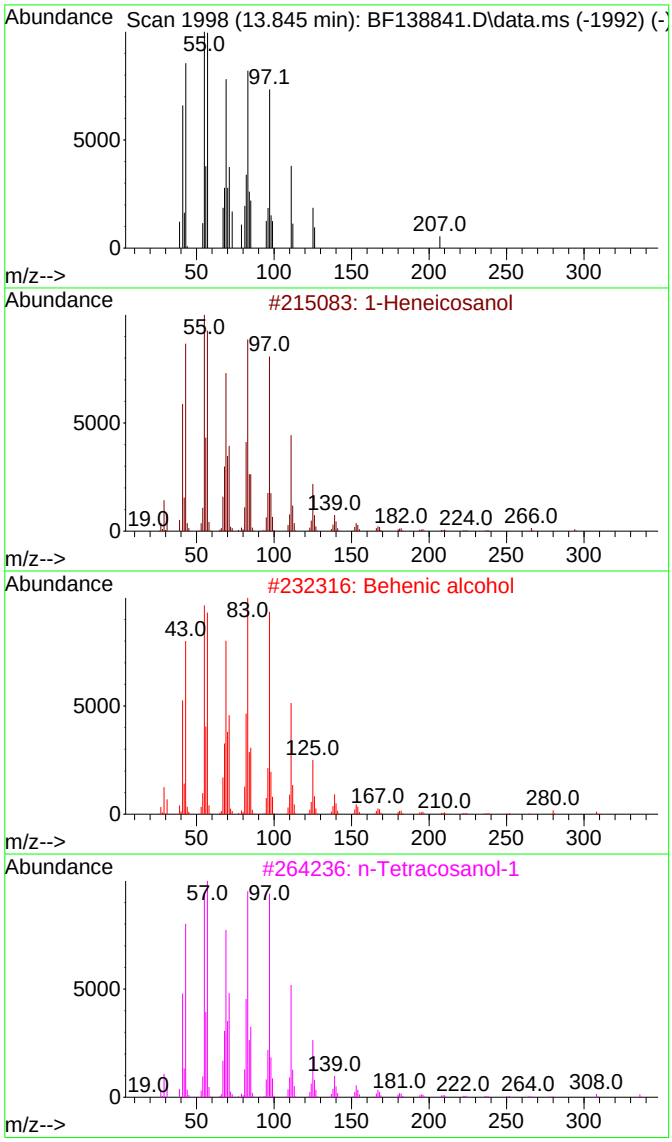
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

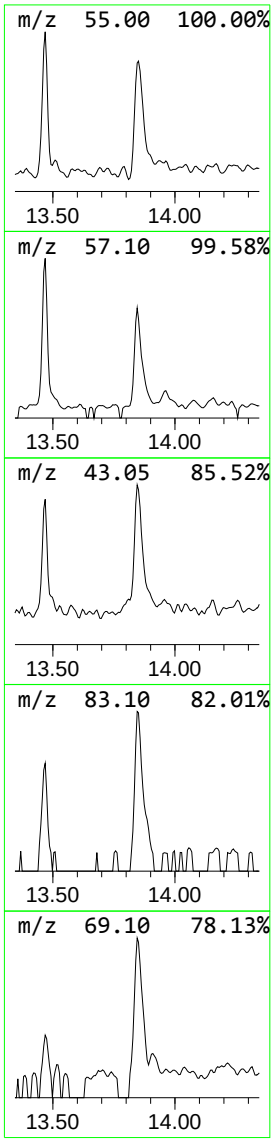
****

Peak Number 7 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	4.39 ng	44095	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

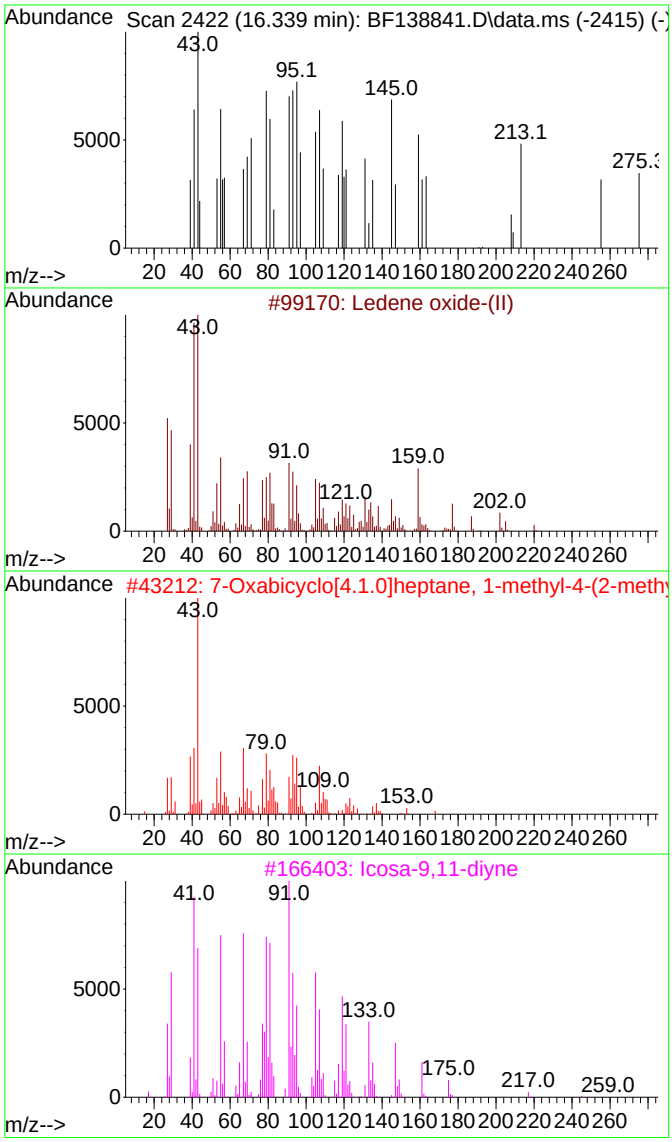
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

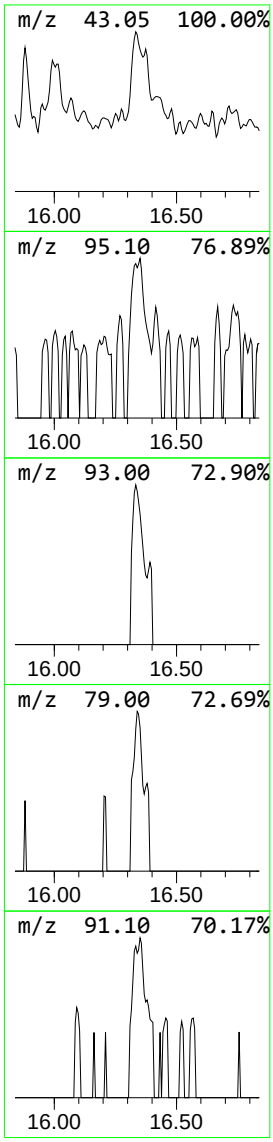
****

Peak Number 8 unknown16.339 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.339	2.73 ng	27679	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ledene oxide-(II)	220	C15H24O	1000159-36-7	32
2	7-Oxabicyclo[4.1.0]heptane, 1-me...	168	C10H16O2	000096-08-2	16
3	Icosa-9,11-diyne	274	C20H34	028393-07-9	14
4	(3R,3aR,4aR,8aR,9aR)-3,8a-Dimeth...	232	C15H20O2	066964-62-3	14
5	7-Hydroxy-3-(1,1-dimethylprop-2-...	230	C14H14O3	056881-08-4	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080724\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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...	2.140	175.9	ng	2263900	1	6.839	257328	20.0
2-Pentanone, 4-...	5.057	2.8	ng	36062	1	6.839	257328	20.0
Cyclohexanone	5.716	2.4	ng	30740	1	6.839	257328	20.0
1-Phenoxypropan...	8.433	3.6	ng	63083	2	8.122	346309	20.0
n-Hexadecanoic ...	11.880	2.4	ng	43764	4	11.357	364152	20.0
Hexanedioic aci...	13.469	3.4	ng	34058	5	13.998	200992	20.0
1-Heneicosanol	13.845	4.4	ng	44095	5	13.998	200992	20.0
unknown16.339	16.339	2.7	ng	27679	6	15.457	202840	20.0