LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111622\
Data File : BF131268.D
Acq On : 16 Nov 2022 16:47
Operator : CG\JU
Sample : N5497-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-13

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-BF111522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	26	34	40	rVB	1580916	2098791	71.00%	11.864%
2	2.393	48	52	59	rVB	49942	67260	2.28%	0.380%
3	4.581	420	424	429	rBV	110122	113955	3.86%	0.644%
4	5.187	522	527	533	rVB	338988	371529	12.57%	2.100%
5	5.575	589	593	597	rVB	1273082	1246418	42.17%	7.046%
6	6.581	759	764	767	rBV	859156	809050	27.37%	4.573%
7	6.975	827	831	834	rVB	589150	522158	17.66%	2.952%
8	7.028	834	840	842	rBV2	29436	34064	1.15%	0.193%
9	7.540	921	927	930	rBV	1735000	1692892	57.27%	9.569%
10	7.857	973	981	990	rBV	35495	40800	1.38%	0.231%
11	8.263	1046	1050	1053	rBV	795590	666814	22.56%	3.769%
12	9.345	1228	1234	1237	rBV	3396882	2956013	100.00%	16.710%
13	10.028	1343	1350	1354	rBV	931218	753819	25.50%	4.261%
14	10.822	1480	1485	1488	rBV	1846130	1619878	54.80%	9.157%
15	11.139	1529	1539	1561	rVB	84700	494327	16.72%	2.794%
16	11.522	1601	1604	1608	rVB	775973	715363	24.20%	4.044%
17	12.045	1689	1693	1696	rBV	61625	62307	2.11%	0.352%
18	12.833	1824	1827	1835	rVB	54830	84542	2.86%	0.478%
19	13.122	1872	1876	1879	rBV	2525187	2223049	75.20%	12.566%
20	14.180	2050	2056	2070	rVB	523665	654082	22.13%	3.697%
21	15.727	2314	2319	2325	rBV	355388	463390	15.68%	2.619%

Sum of corrected areas: 17690501

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Instrument :
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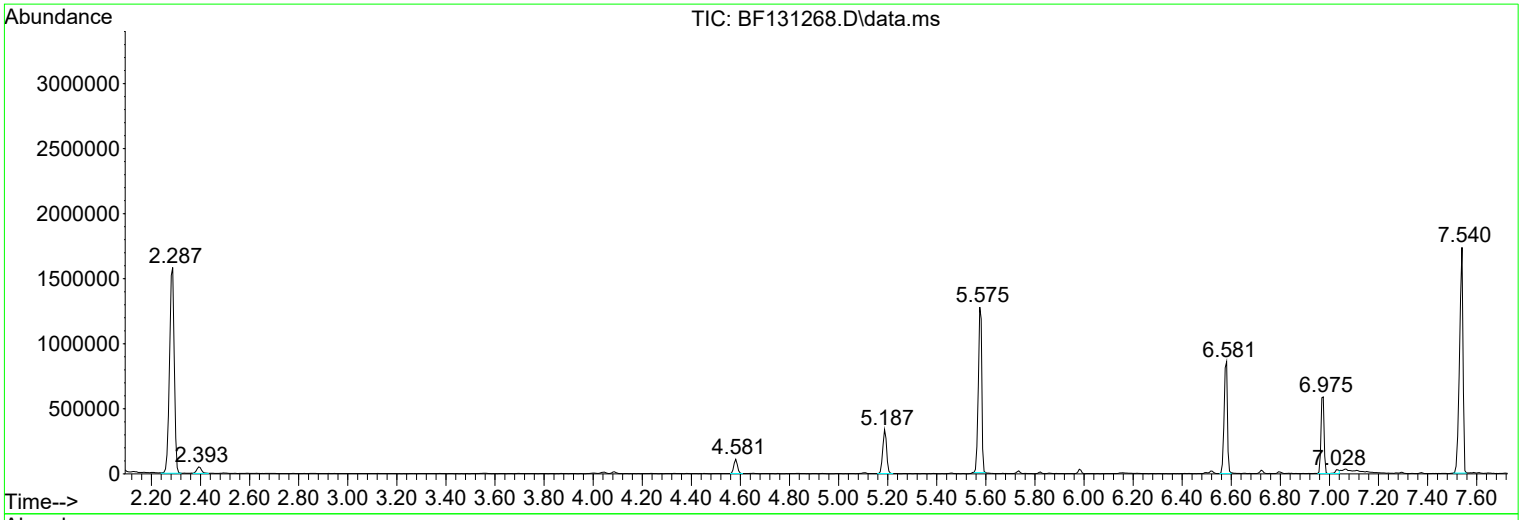
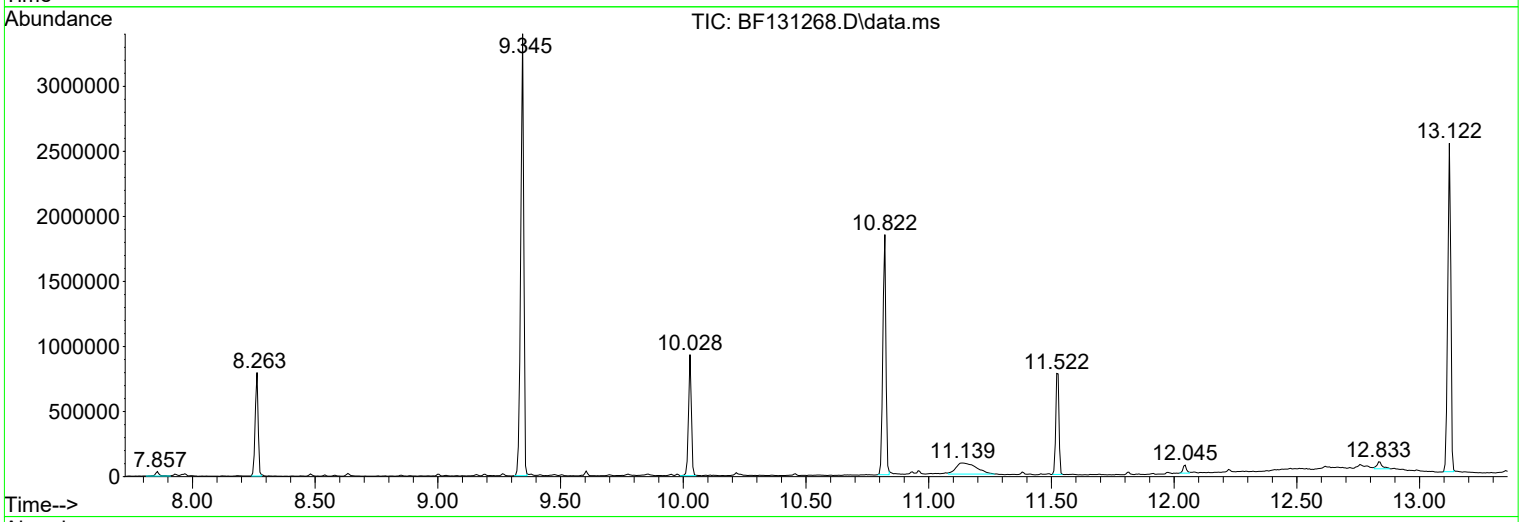
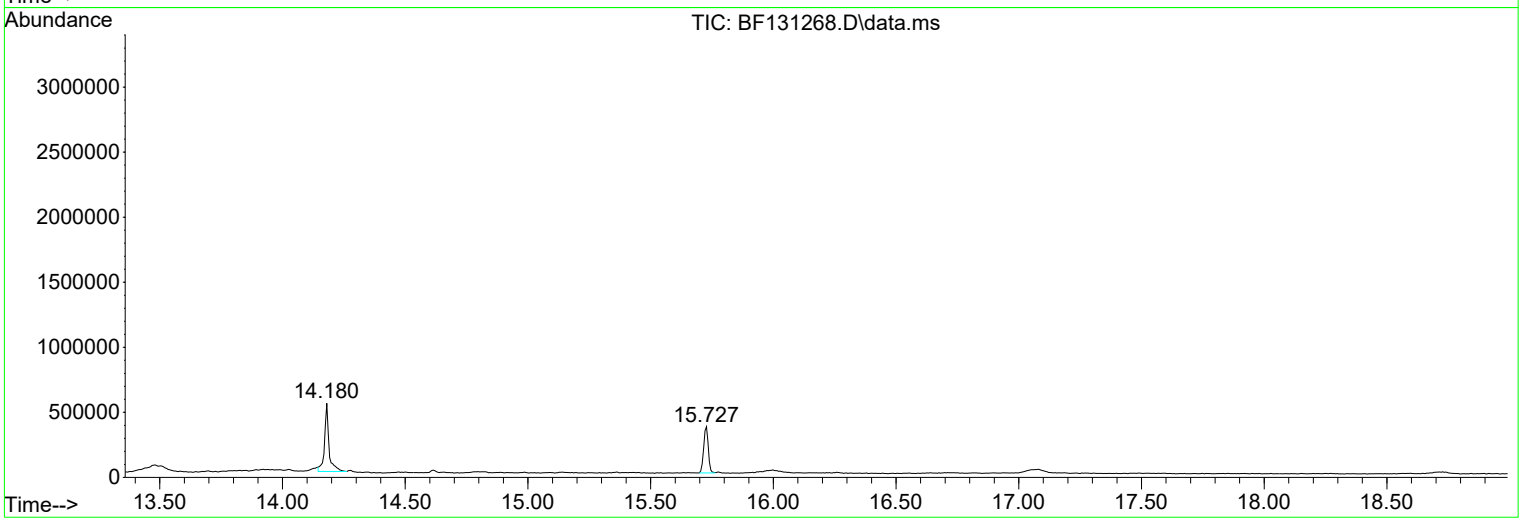
ClientSampleId :
MW-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.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

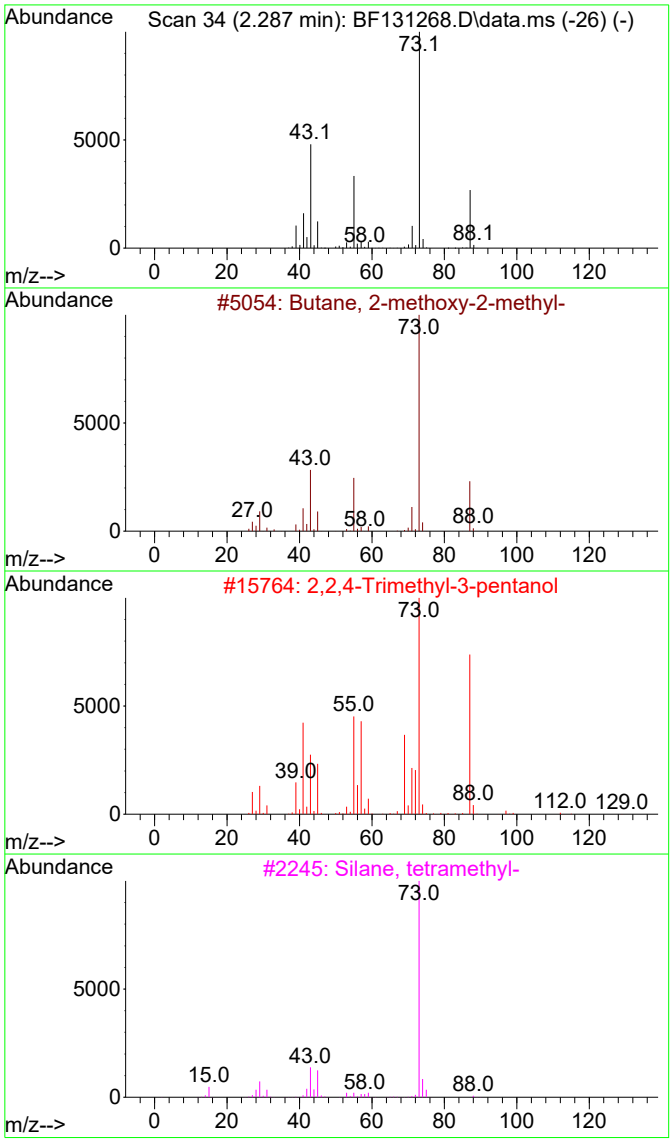
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

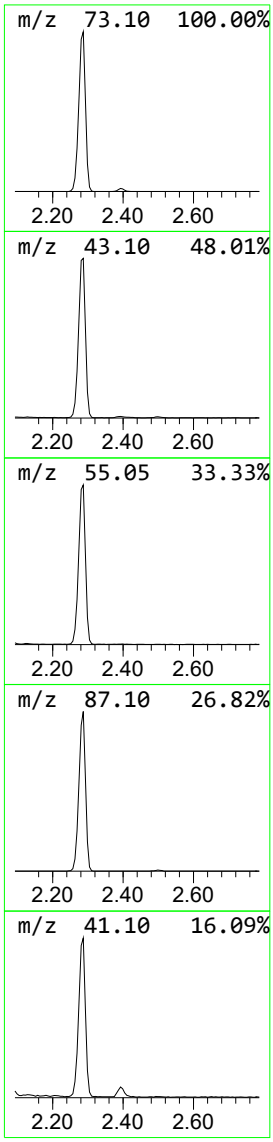
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	80.39 ng	2098790	1,4-Dichlorobenzene-d4	6.975

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12





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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

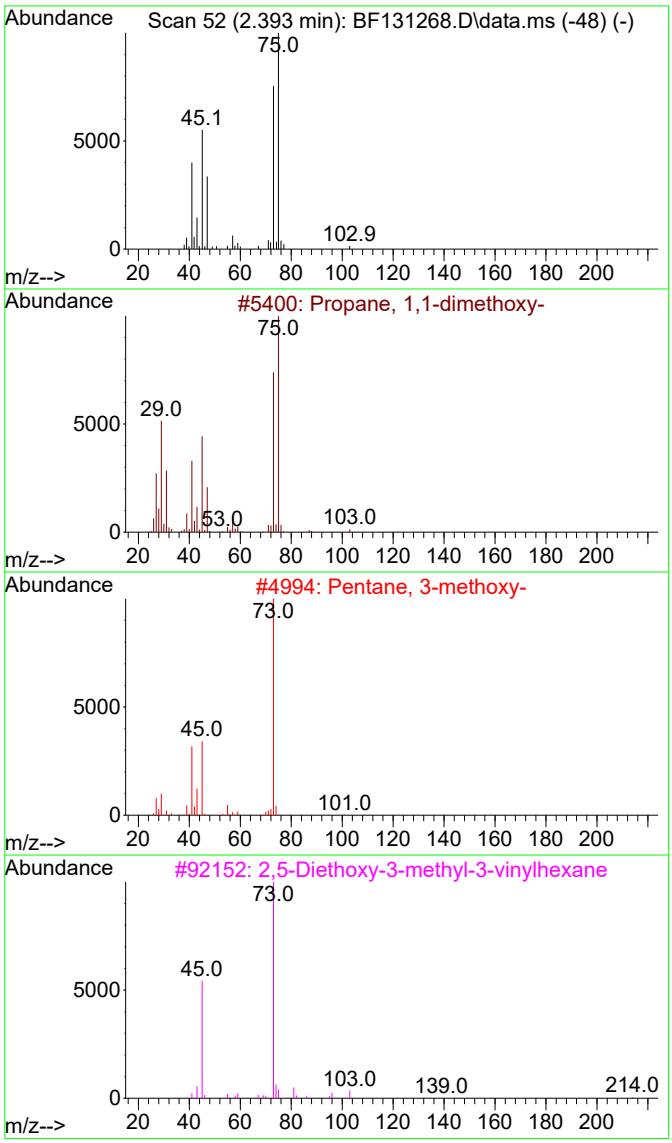
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

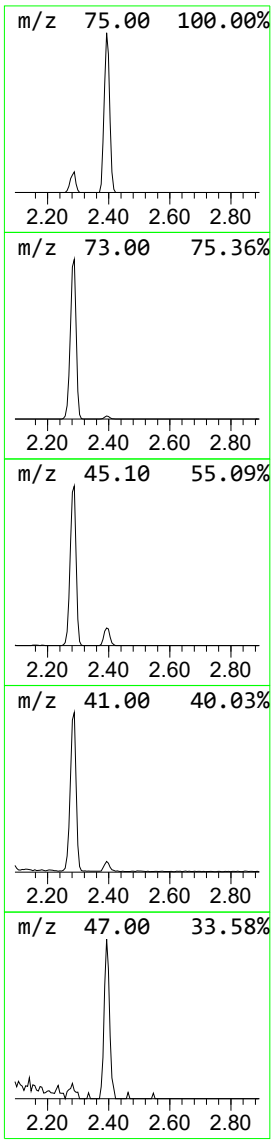
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.393	2.58 ng	67260	1,4-Dichlorobenzene-d4	6.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	10
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9





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Sample : N5497-05
Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-13

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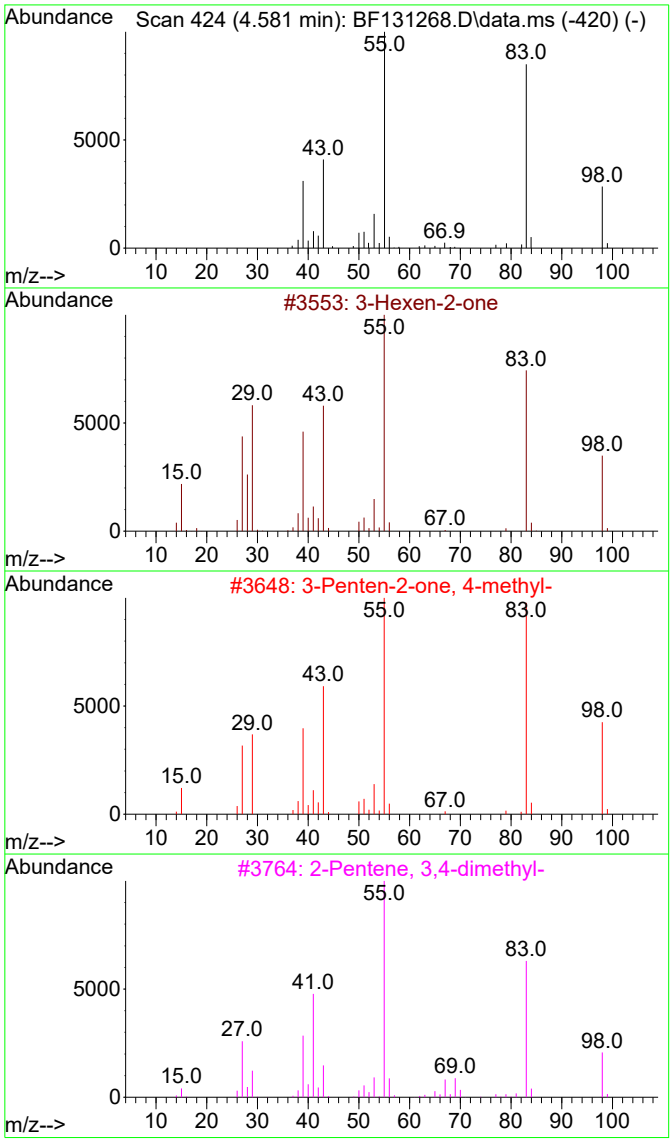
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

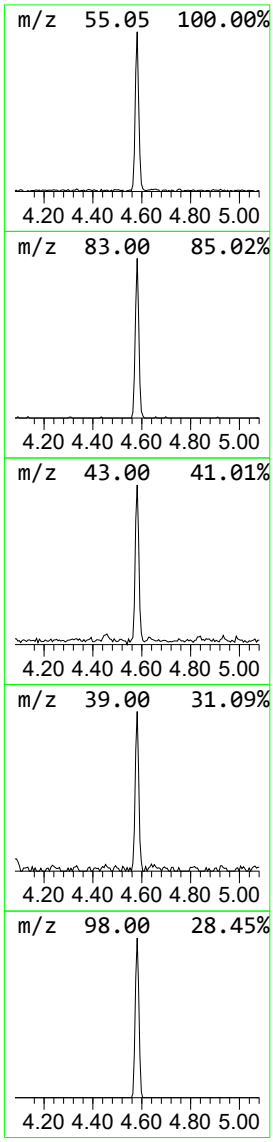
****

Peak Number 3 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.581	4.36 ng	113955	1,4-Dichlorobenzene-d4	6.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Operator : CG\JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.M
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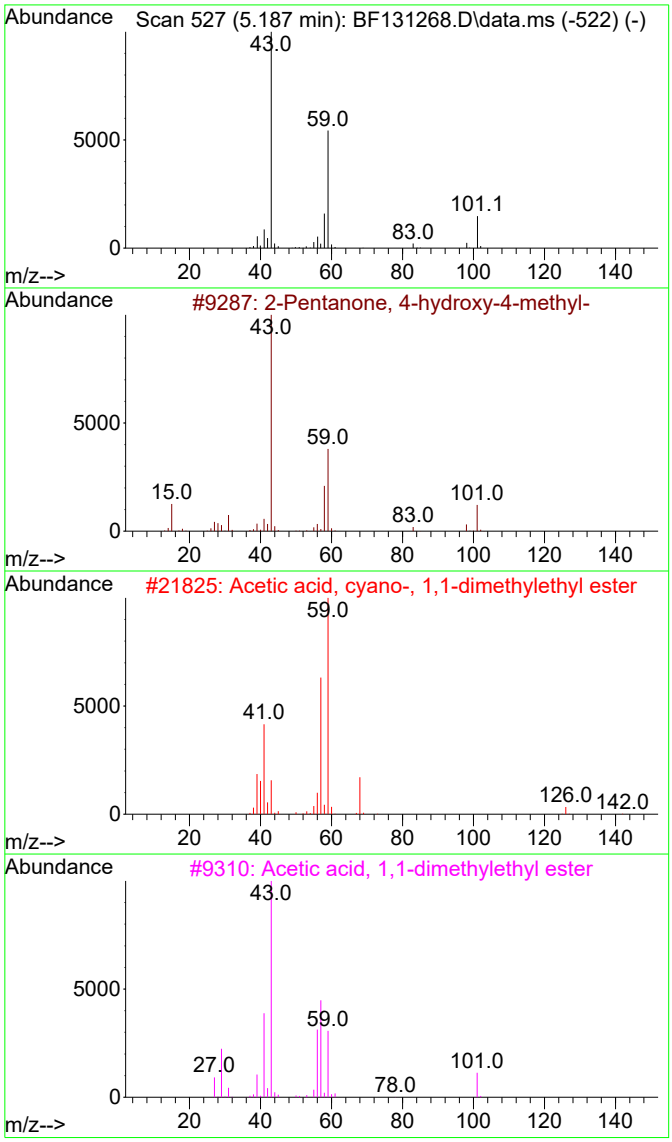
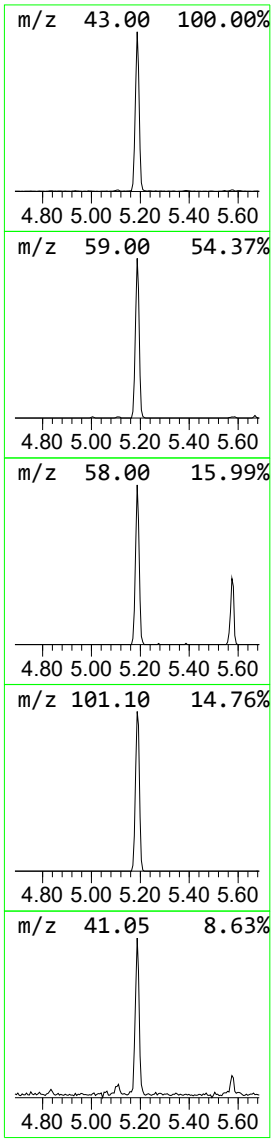
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	14.23 ng	371529	1,4-Dichlorobenzene-d4	6.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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ClientSampleId :
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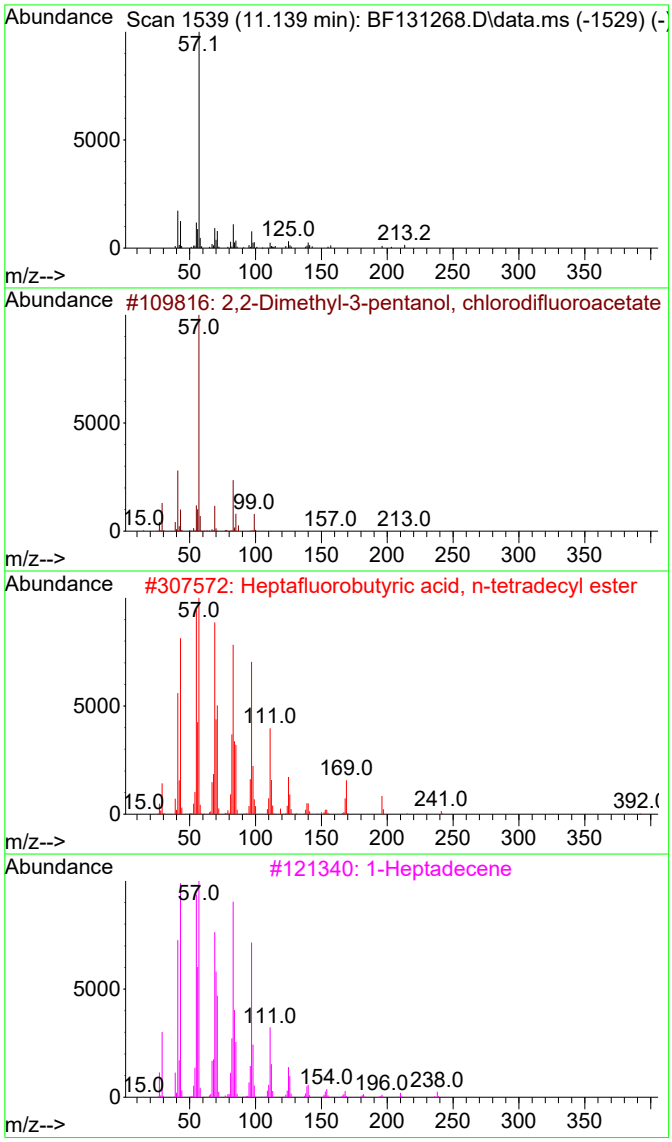
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

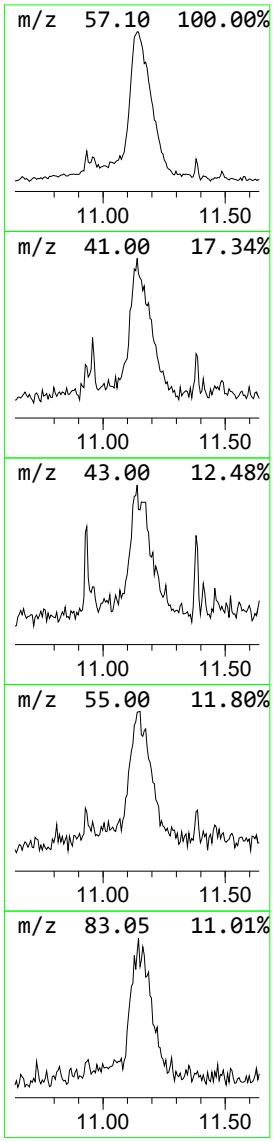
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,2-Dimethyl-3-pentanol, ch... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.139	13.82 ng	494327	Phenanthrene-d10	11.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	53
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	47
3	1-Heptadecene	238	C17H34	006765-39-5	47
4	Butyl tetradecyl ether	270	C18H38O	1000406-40-4	47
5	1-Hexadecanol, 3,7,11,15-tetrame...	298	C20H42O	000645-72-7	43





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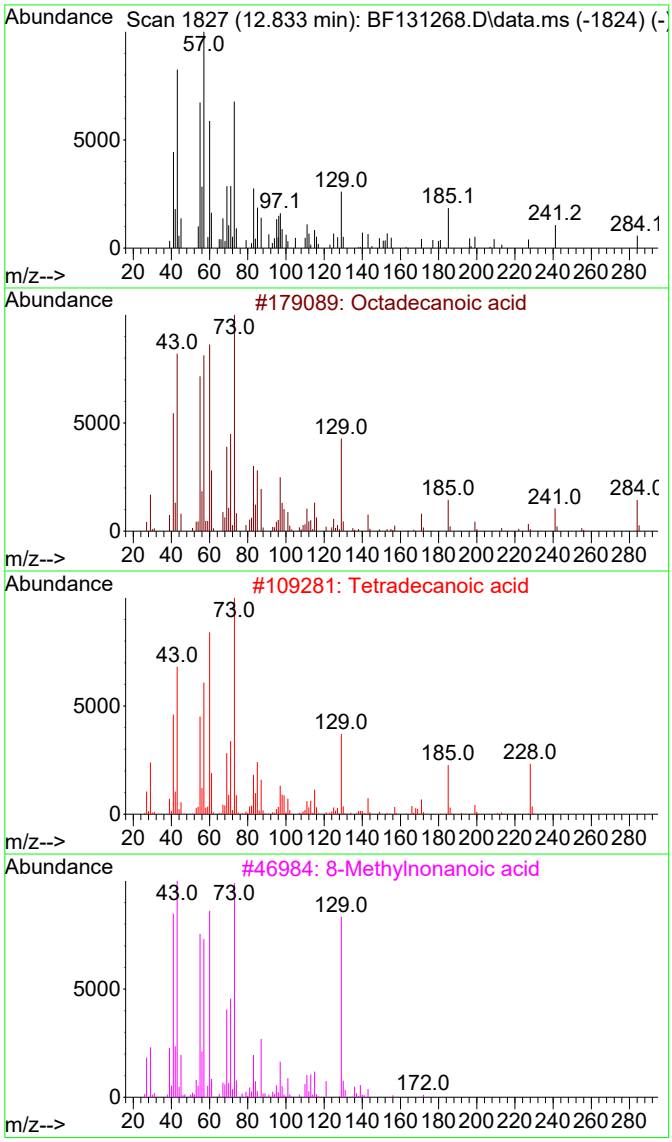
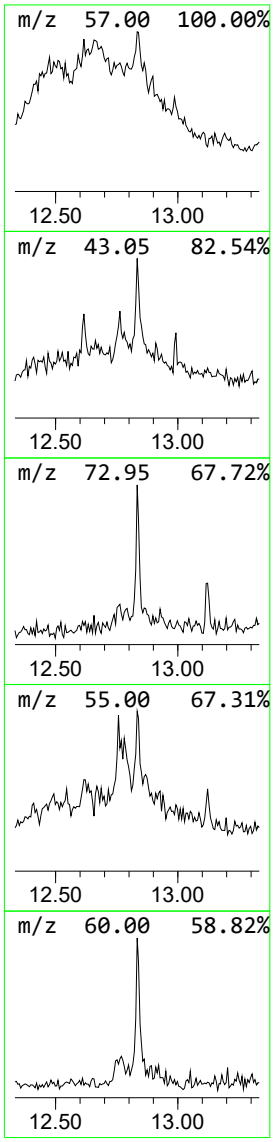
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.833	2.36 ng	84542	Phenanthrene-d10	11.528

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	52
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38
4	Dodecanoic acid	200	C12H24O2	000143-07-7	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	35





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...	2.287	80.4	ng	2098790	1	6.975	522158	20.0
Propane, 1,1-di...	2.393	2.6	ng	67260	1	6.975	522158	20.0
3-Hexen-2-one	4.581	4.4	ng	113955	1	6.975	522158	20.0
2-Pentanone, 4-...	5.187	14.2	ng	371529	1	6.975	522158	20.0
2,2-Dimethyl-3-...	11.139	13.8	ng	494327	4	11.528	715363	20.0
Octadecanoic acid	12.833	2.4	ng	84542	4	11.528	715363	20.0