LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
Data File : BF134066.D
Acq On : 30 Jun 2023 23:05
Operator : CG\JU
Sample : 03358-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1-(0-2)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134066.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	10	20	rVB	1267213	1696560	64.71%	8.876%
2	2.257	25	29	41	rVB2	22686	42569	1.62%	0.223%
3	5.093	507	511	520	rBV	75824	95329	3.64%	0.499%
4	5.481	573	577	588	rBV	2164455	2175229	82.97%	11.380%
5	6.481	742	747	750	rBV	2195004	2173142	82.89%	11.369%
6	6.845	805	809	818	rBV	807893	640321	24.42%	3.350%
7	7.410	900	905	908	rBV	1614180	1432680	54.65%	7.496%
8	8.122	1023	1026	1039	rBV	973690	848958	32.38%	4.442%
9	9.204	1206	1210	1213	rBV	3029385	2621619	100.00%	13.716%
10	9.880	1321	1325	1329	rBV	1043103	902074	34.41%	4.719%
11	10.598	1444	1447	1456	rBV	615413	515458	19.66%	2.697%
12	10.675	1456	1460	1471	rBV	1687210	1499164	57.18%	7.843%
13	10.910	1496	1500	1503	rBV	109347	91136	3.48%	0.477%
14	11.375	1575	1579	1582	rBV	938623	851993	32.50%	4.457%
15	11.398	1582	1583	1587	rVB	52438	34985	1.33%	0.183%
16	11.904	1667	1669	1678	rBV3	106952	120529	4.60%	0.631%
17	12.598	1780	1787	1791	rBV	62577	62064	2.37%	0.325%
18	12.827	1821	1826	1831	rVB	48676	47378	1.81%	0.248%
19	12.974	1847	1851	1854	rBV	2140884	1843512	70.32%	9.645%
20	13.904	2003	2009	2022	rBV4	69472	179693	6.85%	0.940%
21	14.033	2027	2031	2035	rBV	573875	579589	22.11%	3.032%
22	14.804	2159	2162	2170	rBV4	50750	77963	2.97%	0.408%
23	15.539	2282	2287	2292	rBV	450148	581914	22.20%	3.044%

Sum of corrected areas: 19113859

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ClientSampleId :
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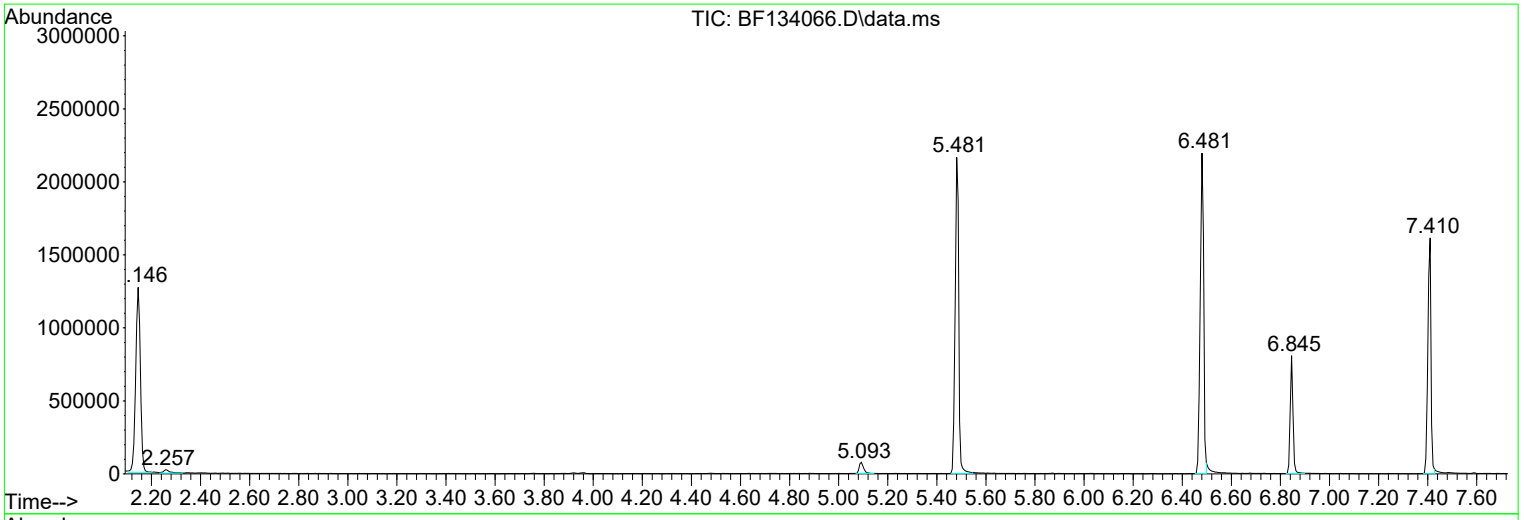
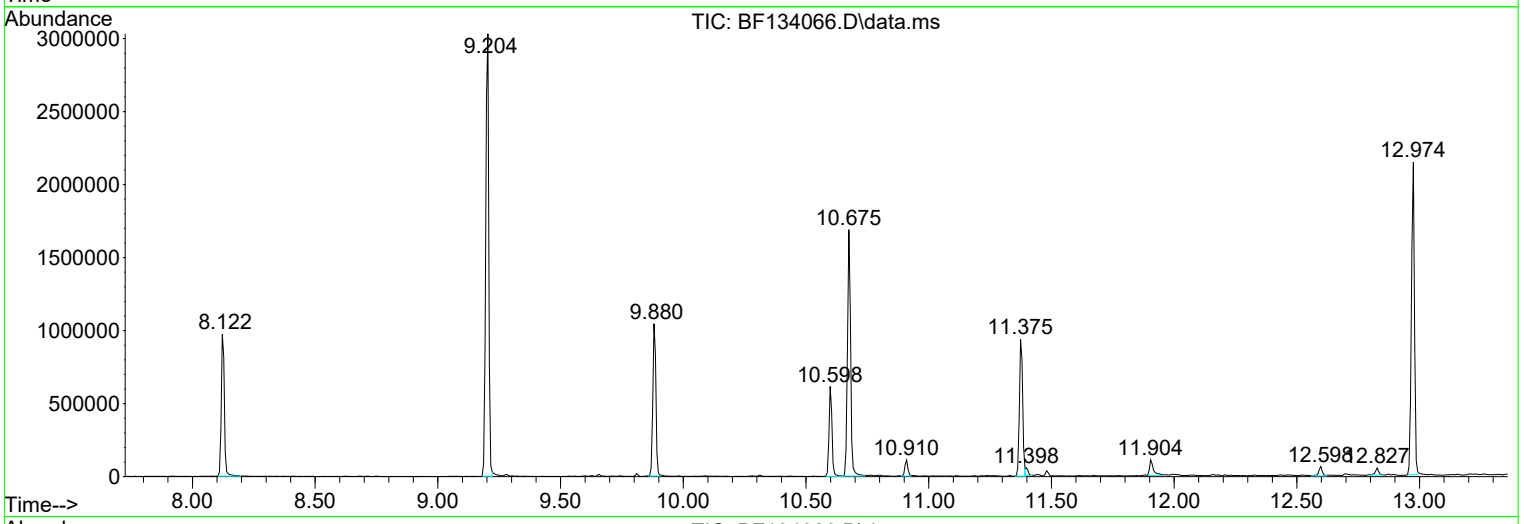
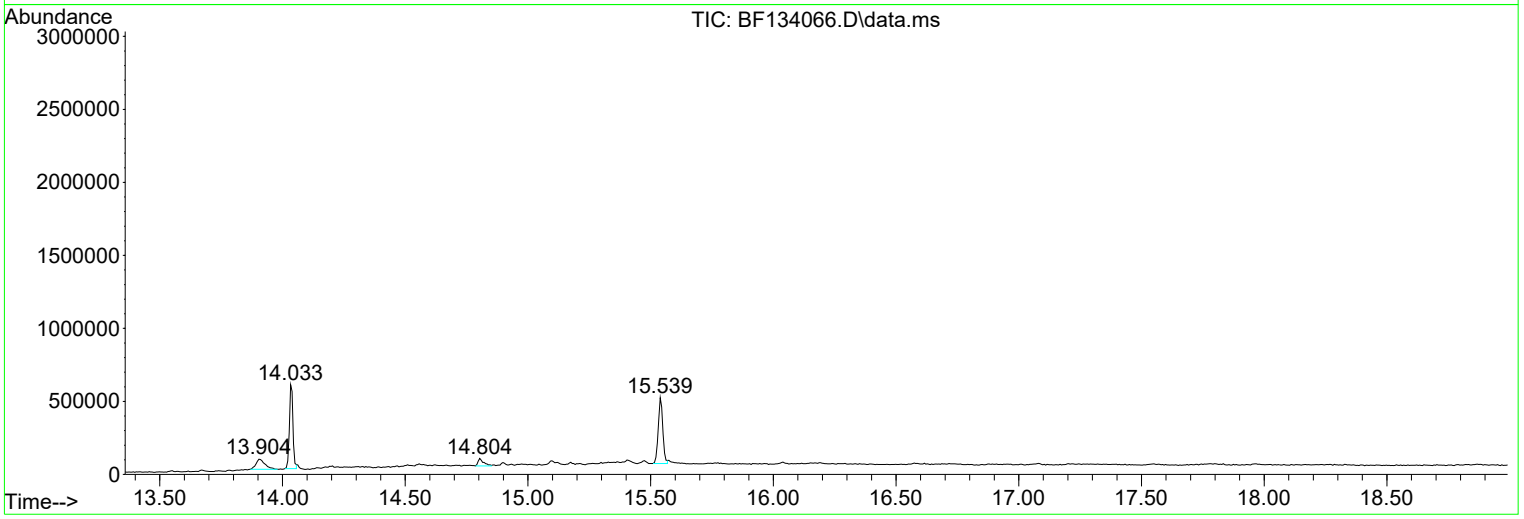
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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
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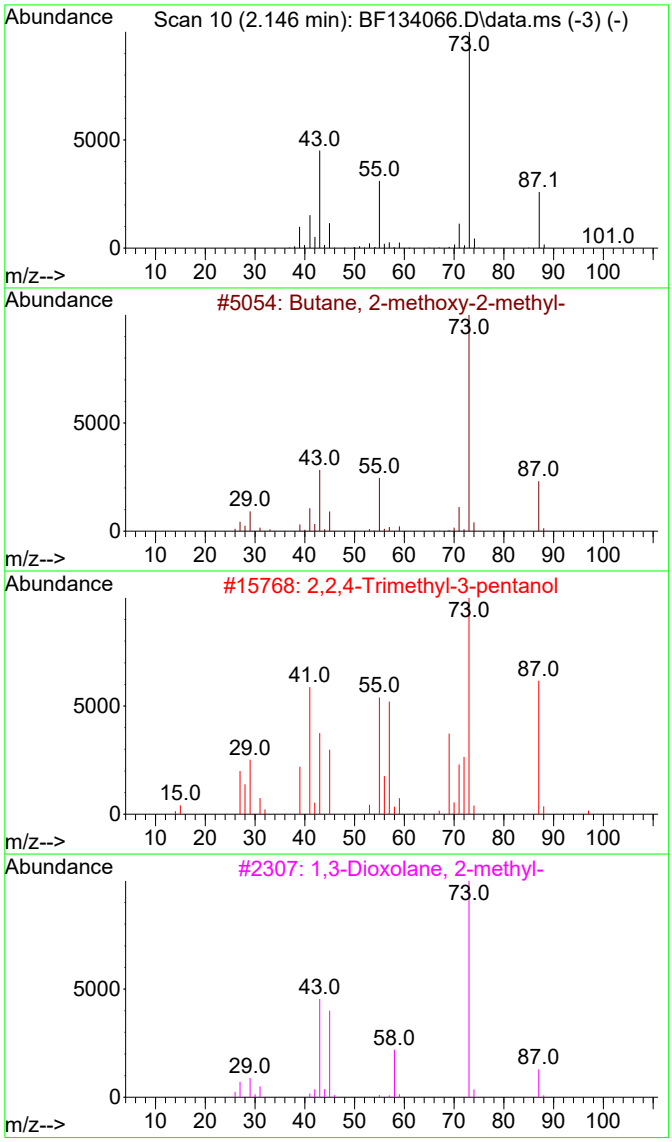
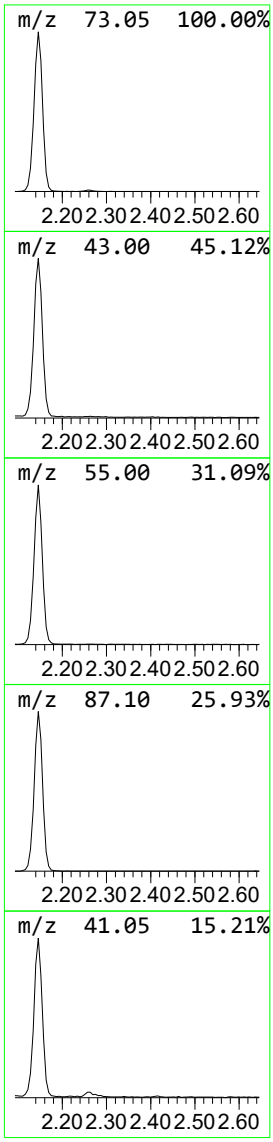
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	52.99 ng	1696560	1,4-Dichlorobenzene-d4	6.845

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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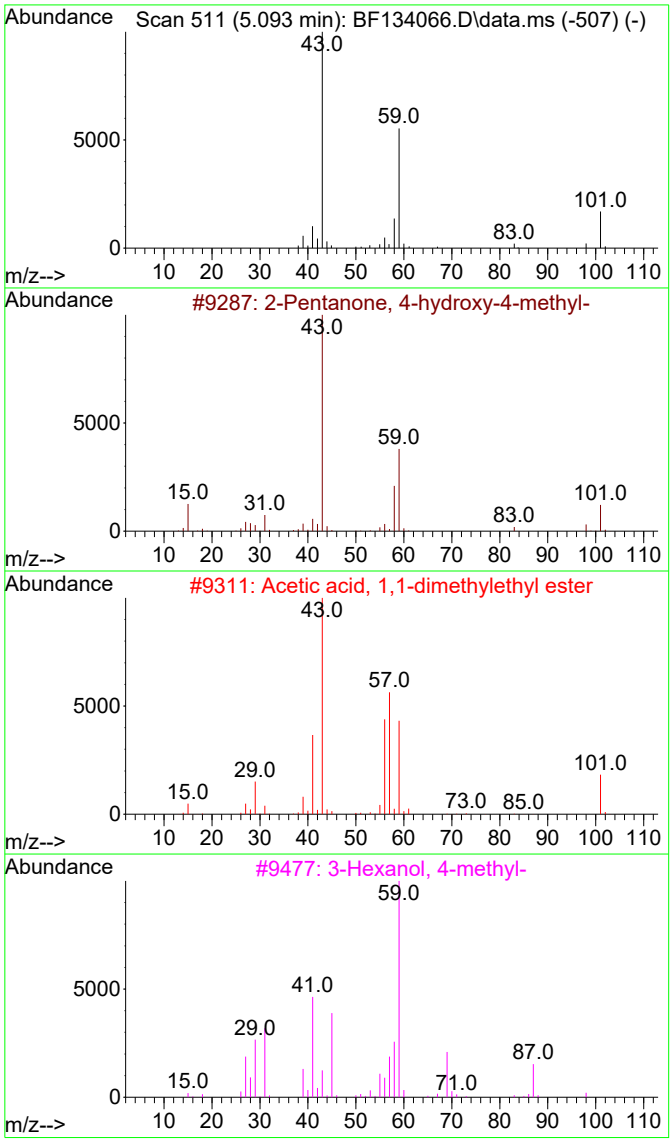
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

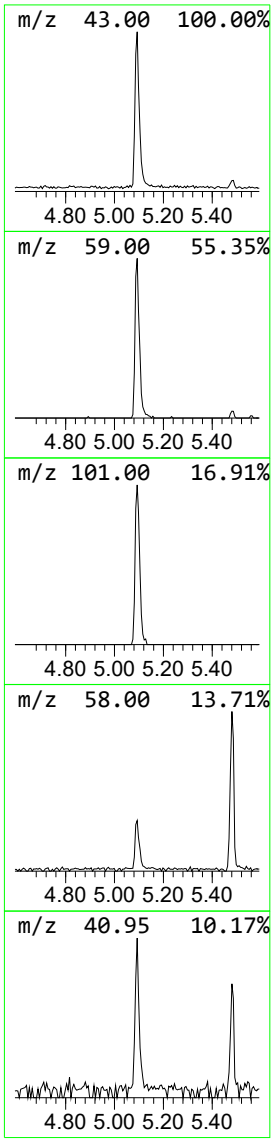
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.98 ng	95329	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





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Operator : CG\JU
Sample : 03358-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

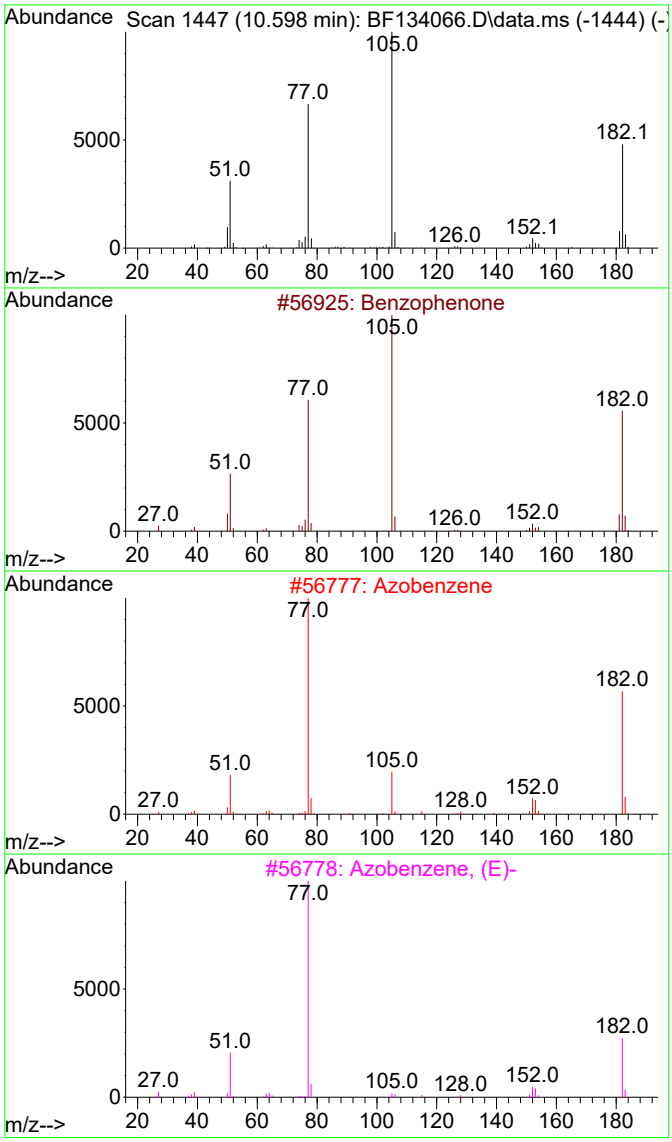
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

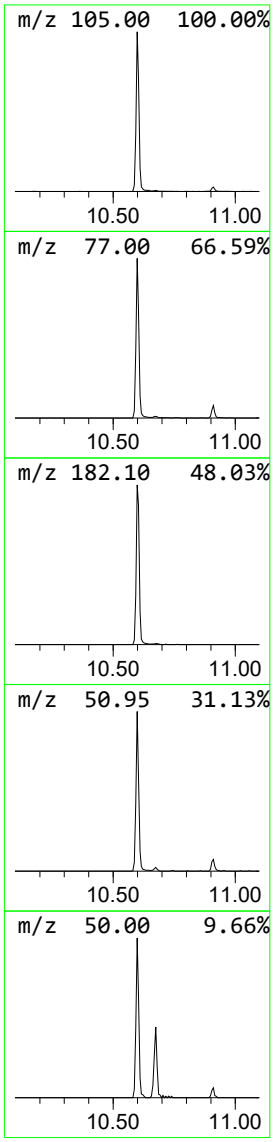
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	11.43 ng	515458	Acenaphthene-d10	9.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	58
3	Azobenzene, (E)-	182	C12H10N2	017082-12-1	53
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
5	Vinyl benzoate	148	C9H8O2	000769-78-8	50





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Instrument :
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ClientSampleId :
SB-1-(0-2)

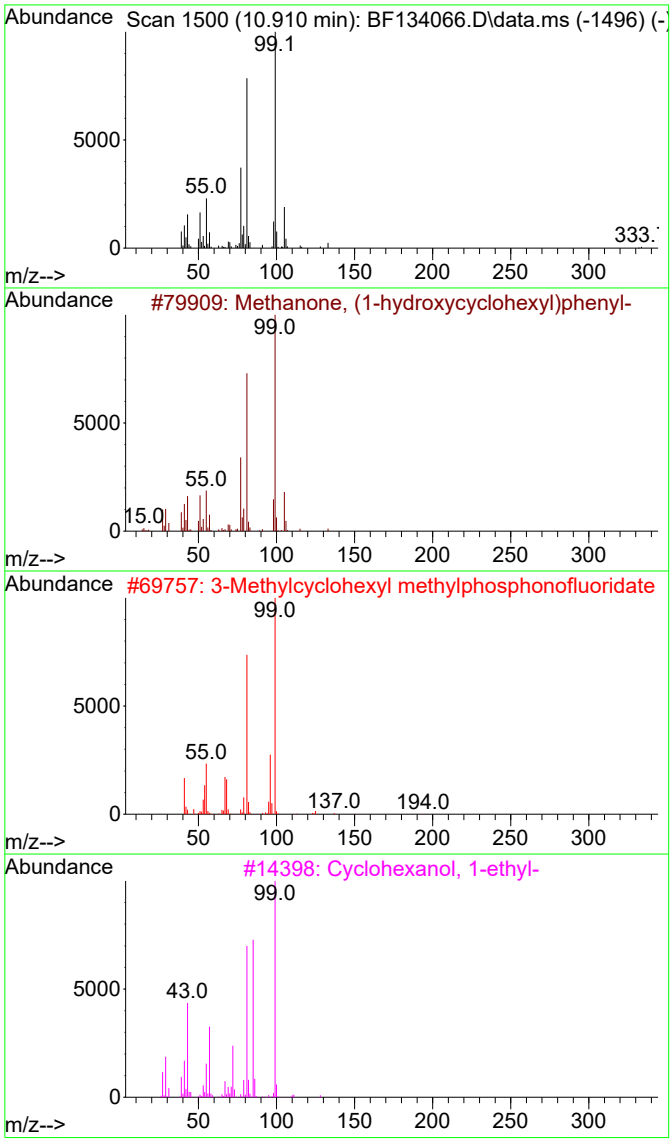
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

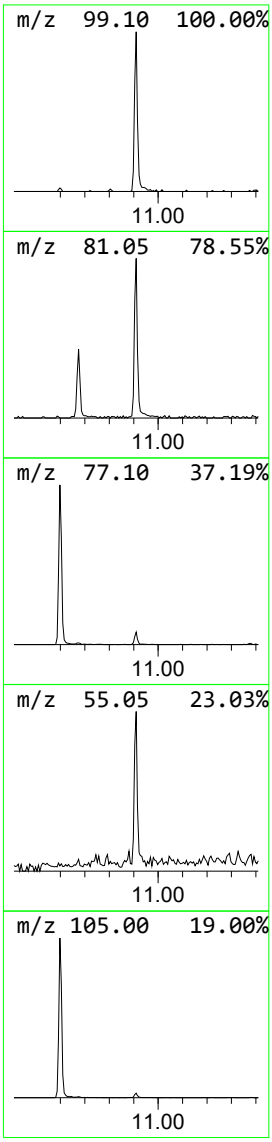
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methanone, (1-hydroxycycloh... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.910	2.14 ng	91136	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2	3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	59
3	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	59
4	Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50
5	2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	42





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ClientSampleId :
SB-1-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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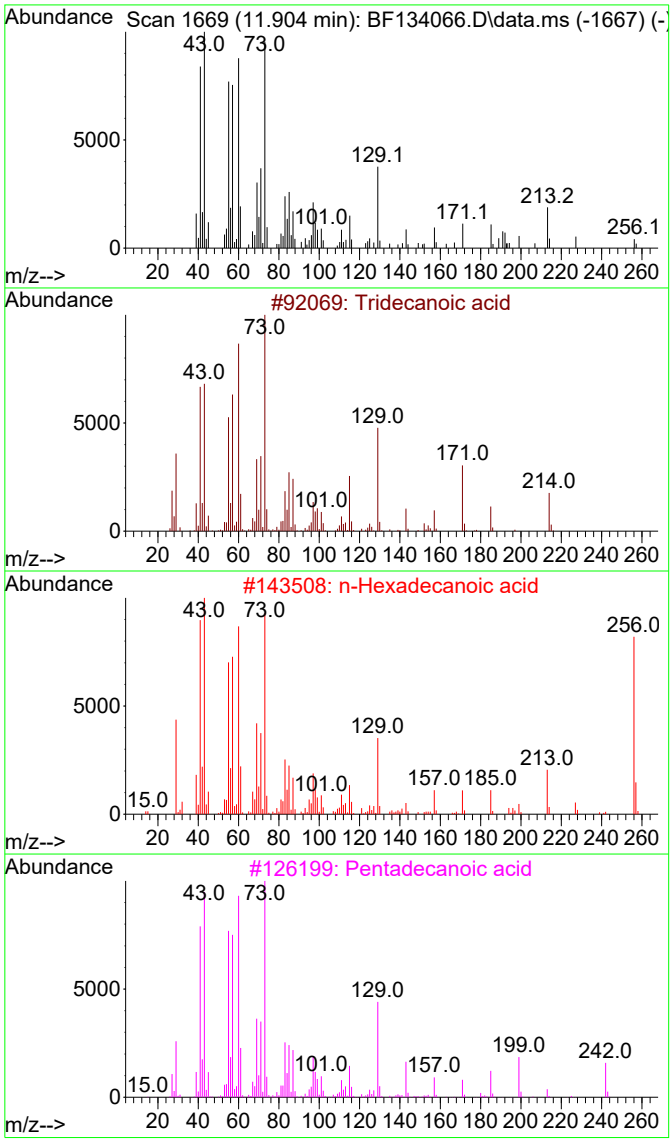
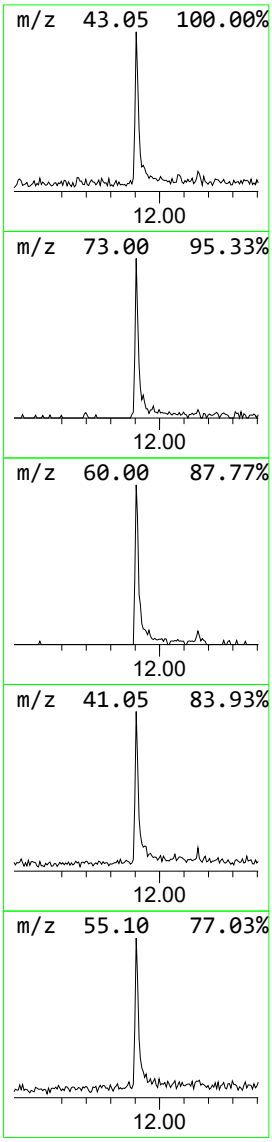
Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.83 ng	120529	Phenanthrene-d10	11.374

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72





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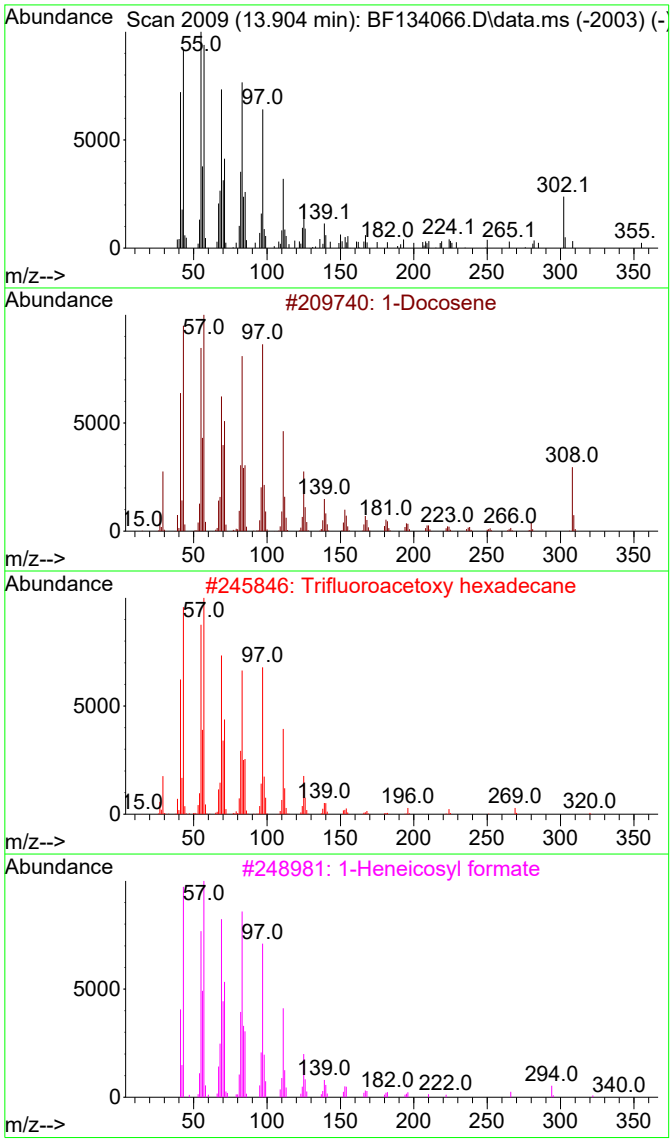
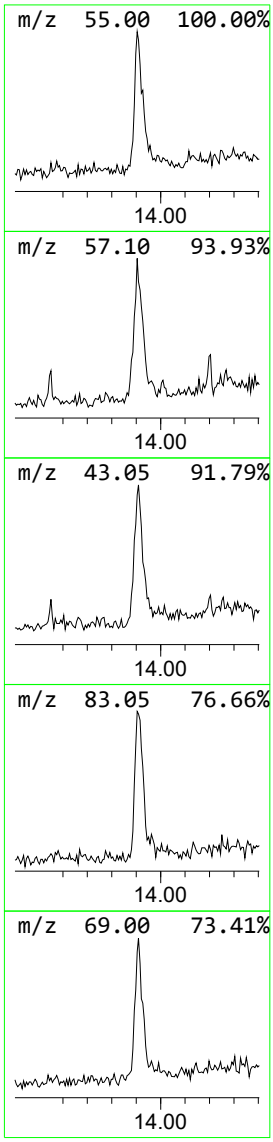
Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	6.20 ng	179693	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	93
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5	1-Tricosene	322	C23H46	018835-32-0	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

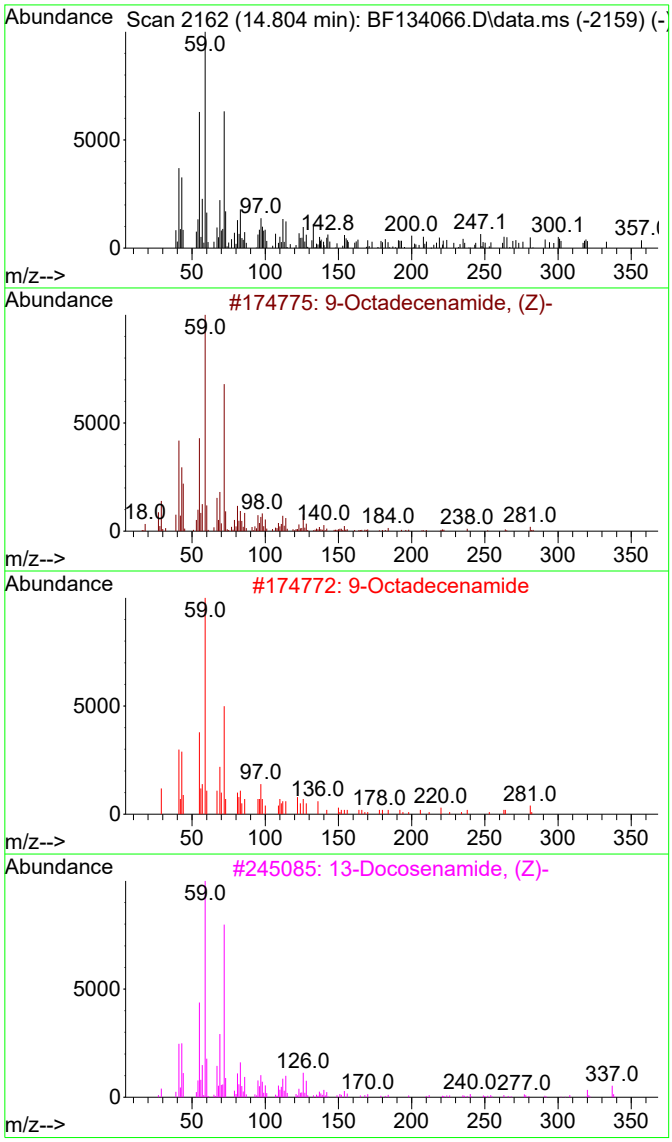
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

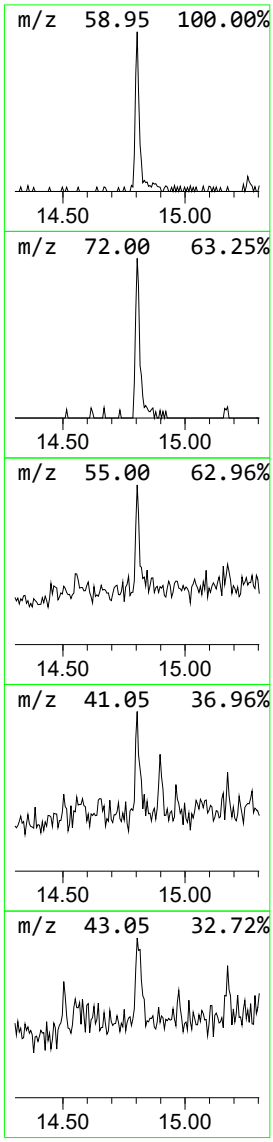
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	2.68 ng	77963	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	9-Octadecenamide	281	C18H35NO	003322-62-1	76
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
4	Octanamide	143	C8H17NO	000629-01-6	59
5	Palmitoleamide	253	C16H31NO	106010-22-4	59





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	53.0	ng	1696560	1	6.845	640321	20.0
2-Pentanone, 4-...	5.093	3.0	ng	95329	1	6.845	640321	20.0
Benzophenone	10.598	11.4	ng	515458	3	9.880	902074	20.0
Methanone, (1-h...	10.910	2.1	ng	91136	4	11.374	851993	20.0
Tridecanoic acid	11.904	2.8	ng	120529	4	11.374	851993	20.0
1-Docosene	13.904	6.2	ng	179693	5	14.033	579589	20.0
9-Octadecenamid...	14.804	2.7	ng	77963	6	15.539	581914	20.0