LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139946.D
Acq On : 22 Oct 2024 23:43
Operator : RC/JU
Sample : P4385-18
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-9

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139946.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	14	24	rVB	1378507	2194305	100.00%	13.190%
2	3.763	279	284	291	rBV	14554	24402	1.11%	0.147%
3	5.104	505	512	518	rVB	90044	125907	5.74%	0.757%
4	5.498	574	579	585	rBV	1226634	1619960	73.83%	9.737%
5	6.504	744	750	755	rBV	1184042	1503255	68.51%	9.036%
6	6.893	810	816	821	rBV	600063	761145	34.69%	4.575%
7	7.445	904	910	915	rBV	823884	1011176	46.08%	6.078%
8	7.698	949	953	958	rBV	34891	42066	1.92%	0.253%
9	8.169	1028	1033	1038	rBV	700840	857169	39.06%	5.152%
10	9.245	1210	1216	1226	rBV	1235991	1547914	70.54%	9.304%
11	9.922	1326	1331	1343	rVB	614756	795846	36.27%	4.784%
12	10.633	1448	1452	1460	rBV	80028	100687	4.59%	0.605%
13	10.710	1460	1465	1479	rVV	659618	838576	38.22%	5.041%
14	11.410	1579	1584	1592	rBV	627417	814545	37.12%	4.896%
15	11.480	1592	1596	1603	rVB3	17948	26441	1.20%	0.159%
16	11.933	1667	1673	1685	rBV	133747	216191	9.85%	1.299%
17	12.622	1786	1790	1795	rBV	72049	98535	4.49%	0.592%
18	12.722	1803	1807	1813	rBV4	20315	37996	1.73%	0.228%
19	12.851	1825	1829	1835	rVB	59517	84294	3.84%	0.507%
20	12.998	1848	1854	1859	rBV	1345219	1747064	79.62%	10.501%
21	13.892	2001	2006	2014	rBV	193304	291462	13.28%	1.752%
22	14.051	2027	2033	2043	rVB	704939	987170	44.99%	5.934%
23	14.521	2110	2113	2118	rBV	39959	53906	2.46%	0.324%
24	15.174	2221	2224	2235	rVB	76121	125384	5.71%	0.754%
25	15.527	2279	2284	2296	rVB	398830	641772	29.25%	3.858%
26	16.015	2363	2367	2372	rVB	58158	89541	4.08%	0.538%

Sum of corrected areas: 16636709

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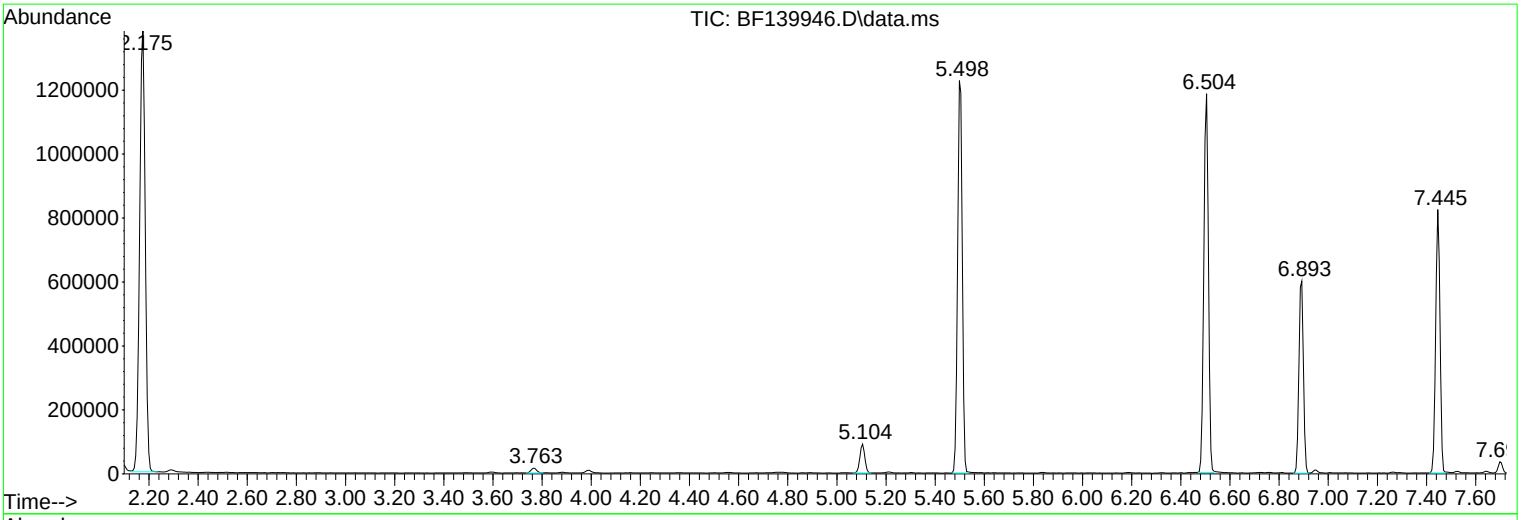
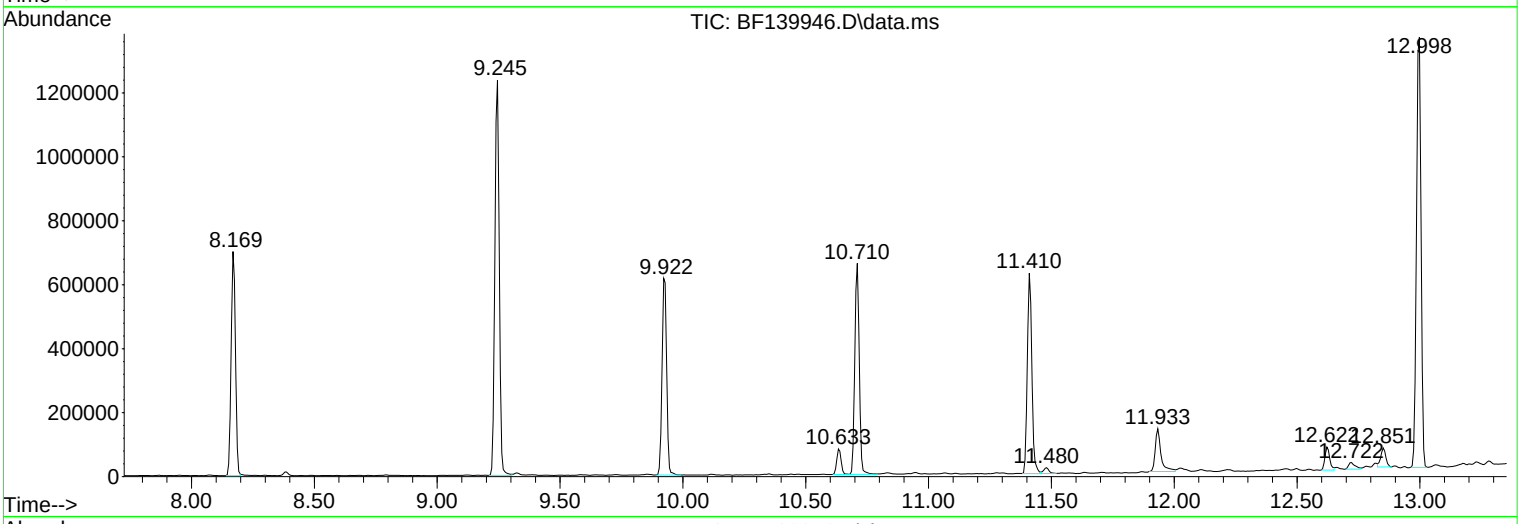
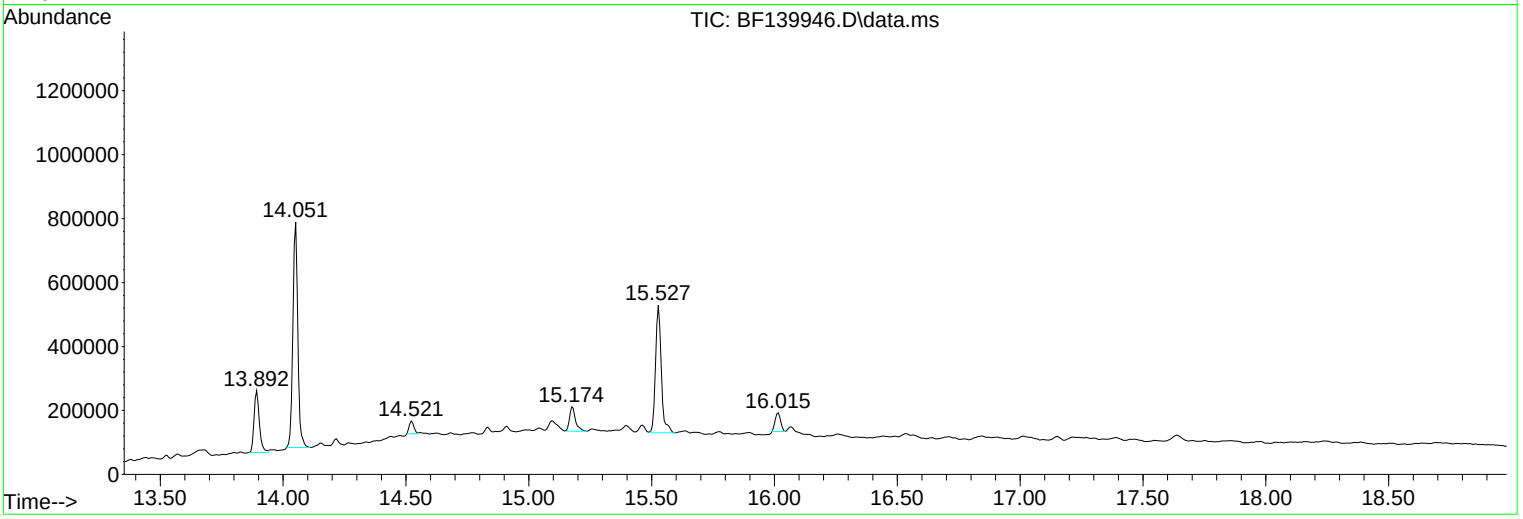
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

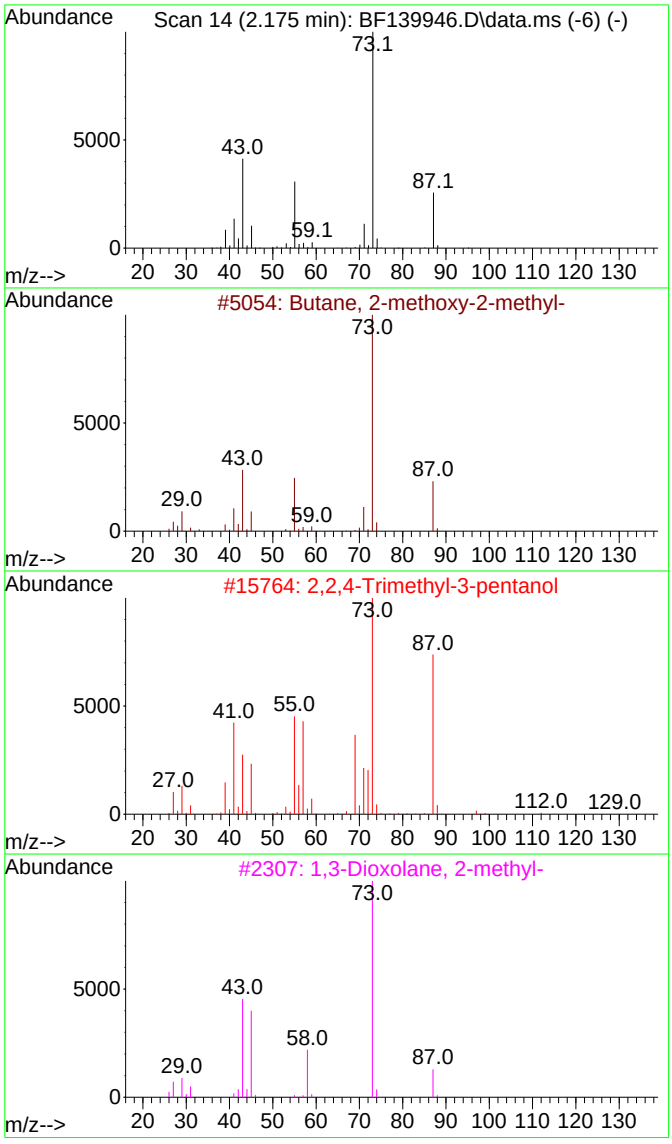
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

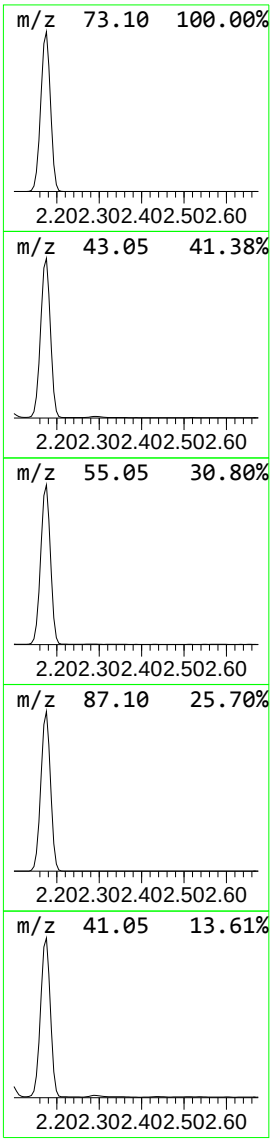
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	57.66 ng	2194310	1,4-Dichlorobenzene-d4	6.893

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	25
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Acq On : 22 Oct 2024 23:43
Operator : RC/JU
Sample : P4385-18
Misc :
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Instrument :
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ClientSampleId :
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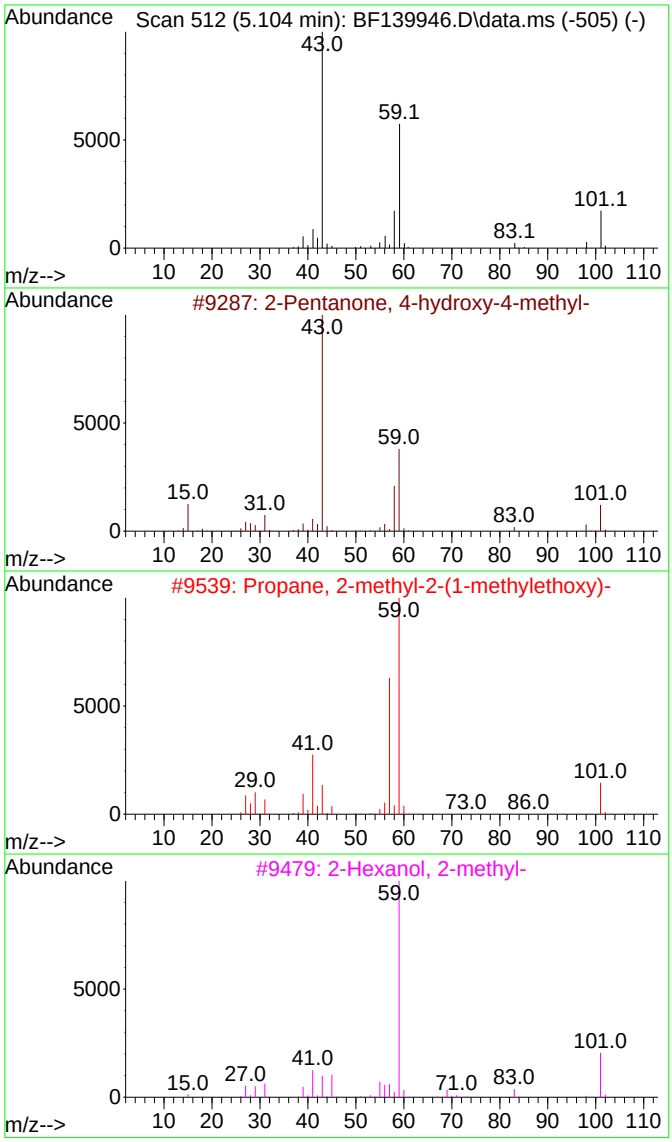
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

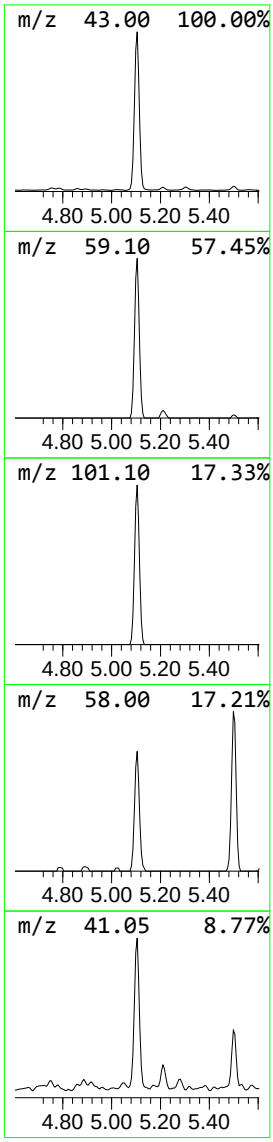
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	3.31 ng	125907	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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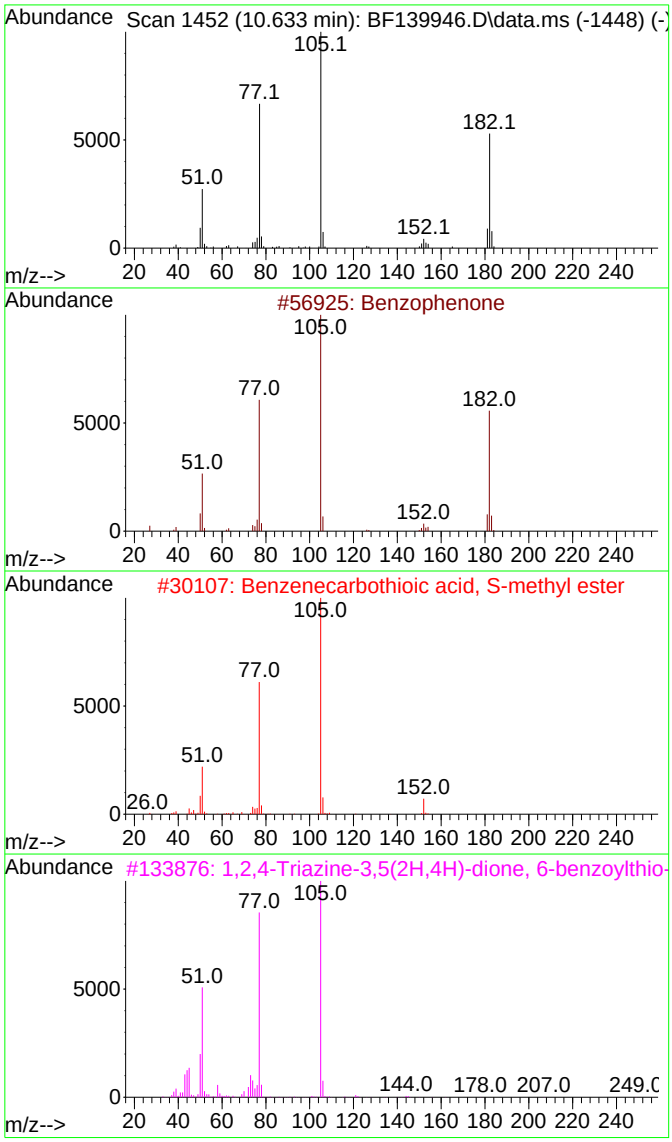
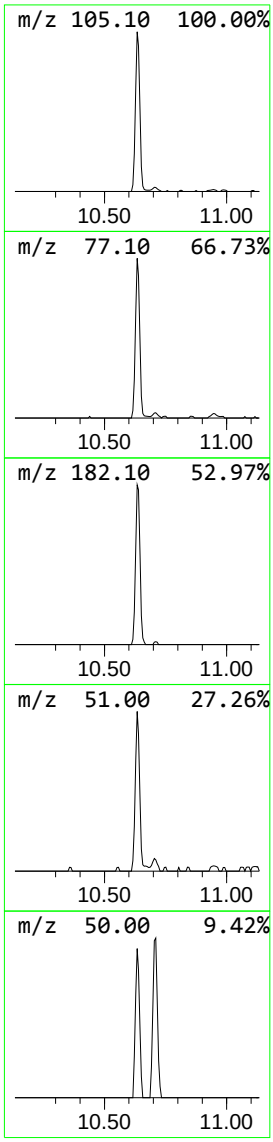
Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.633	2.53 ng	100687	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	47
4	5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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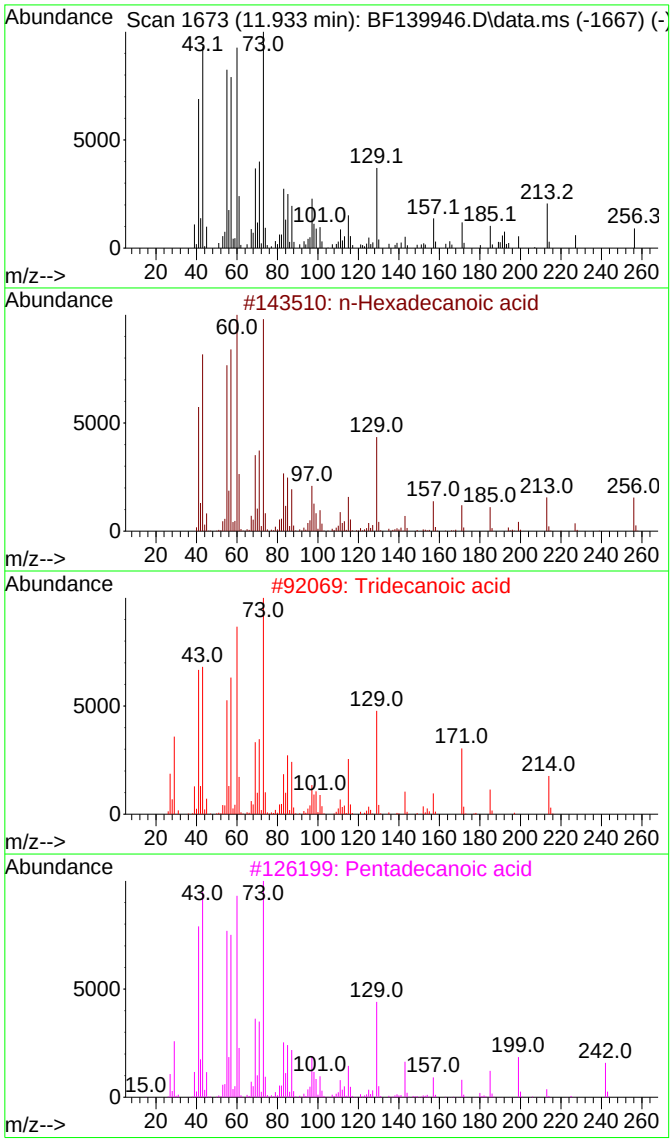
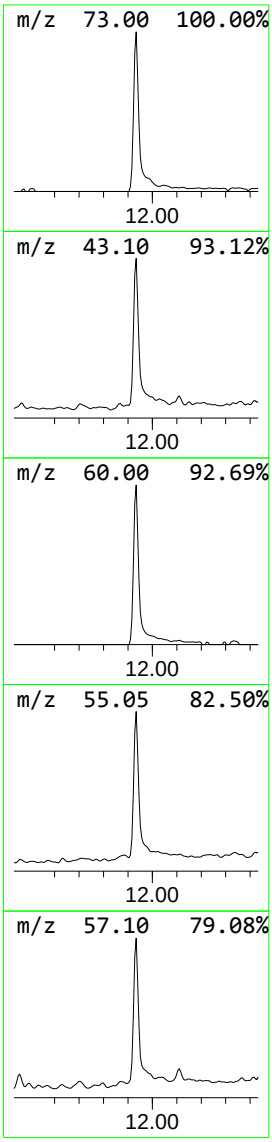
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	5.31 ng	216191	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

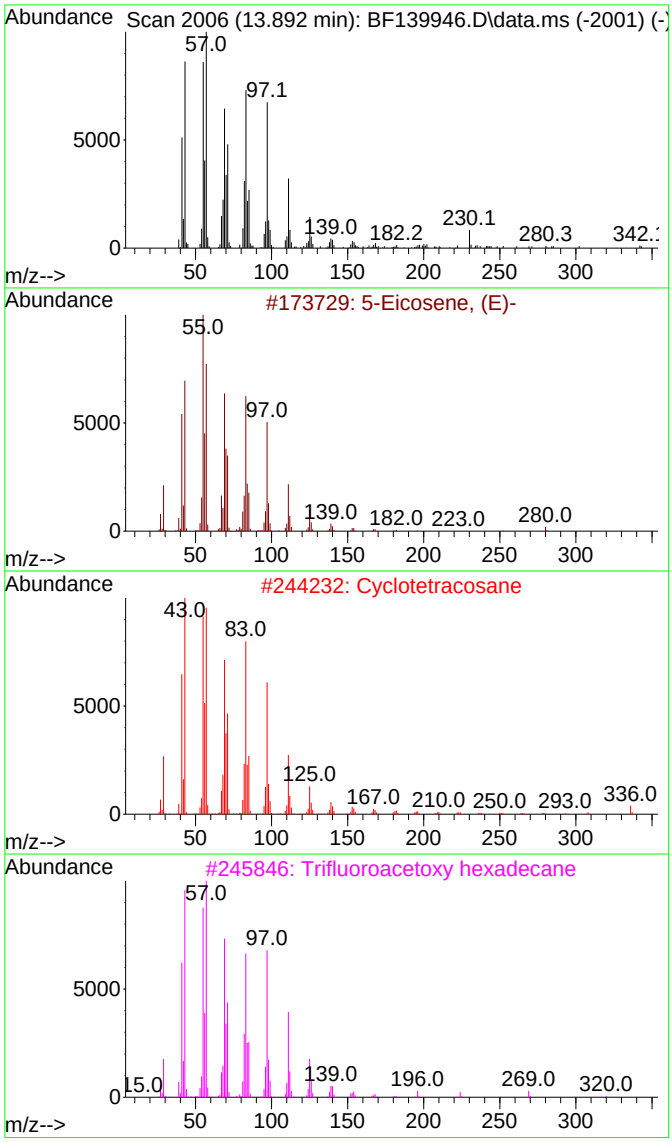
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

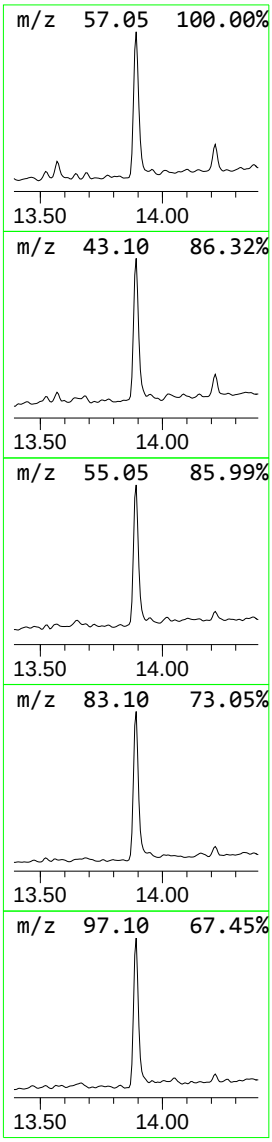
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.91 ng	291462	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Cyclotetracosane	336	C24H48	000297-03-0	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5	1-Docosene	308	C22H44	001599-67-3	94





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TIC Library : C:\Database\NIST20.L
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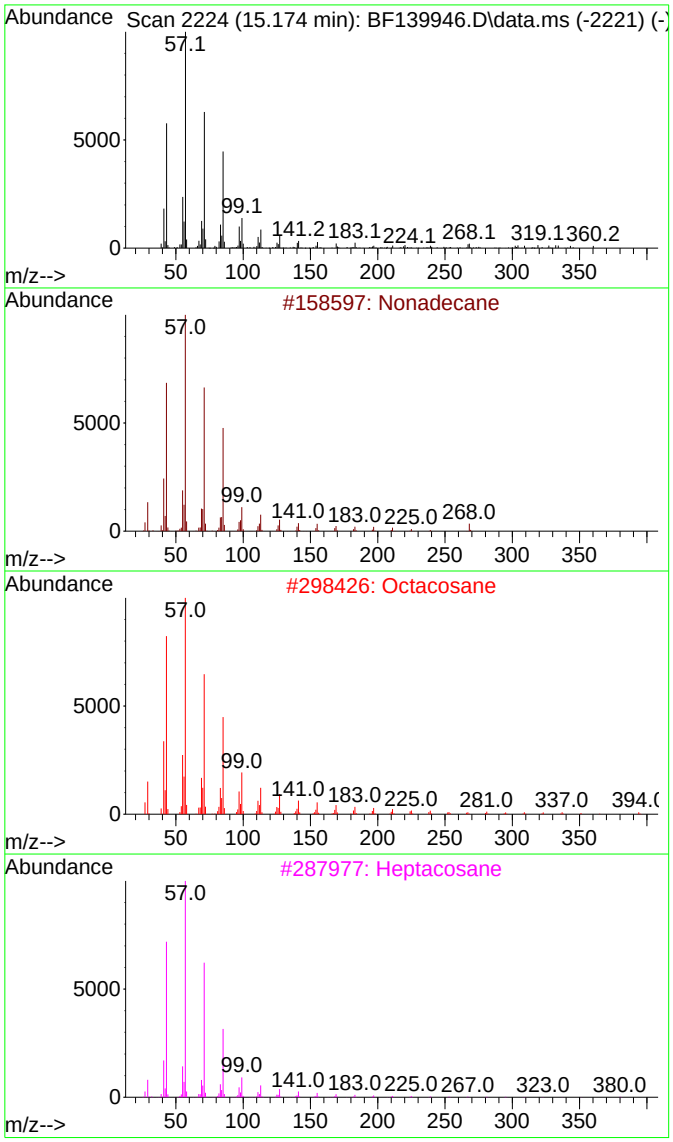
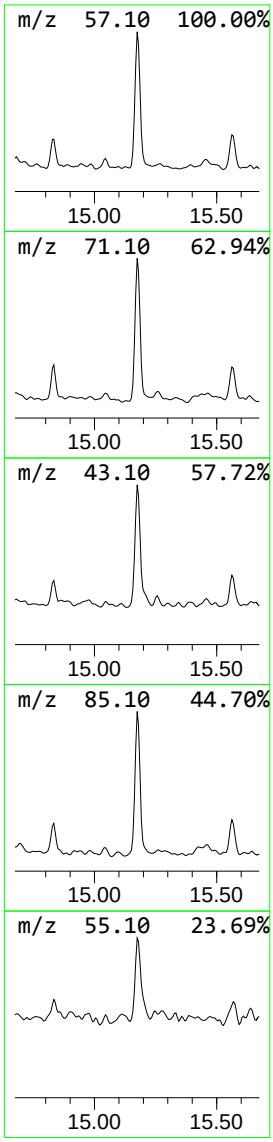
Peak Number 6 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	3.91 ng	125384	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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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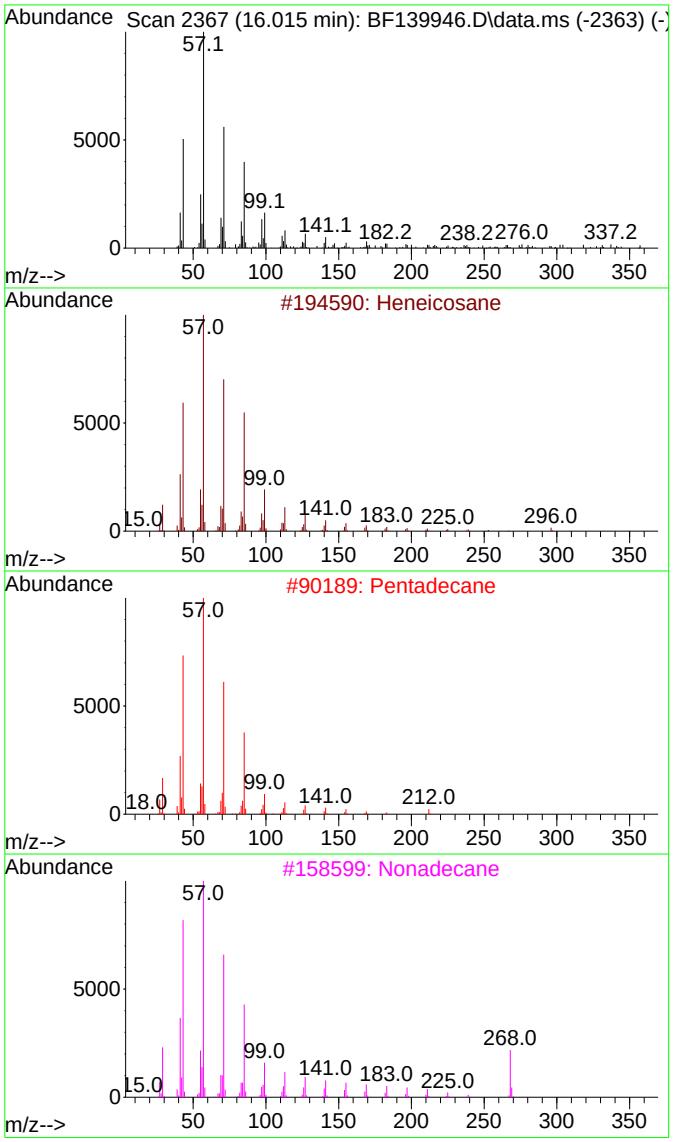
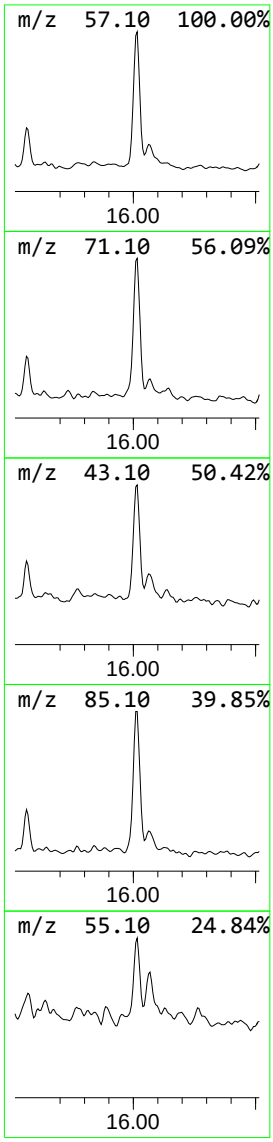
Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	2.79 ng	89541	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Pentadecane	212	C15H32	000629-62-9	93
3	Nonadecane	268	C19H40	000629-92-5	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Hexacosane	366	C26H54	000630-01-3	90





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...	2.175	57.7	ng	2194310	1	6.893	761145	20.0
2-Pentanone, 4-...	5.104	3.3	ng	125907	1	6.893	761145	20.0
Benzophenone	10.633	2.5	ng	100687	3	9.922	795846	20.0
n-Hexadecanoic ...	11.933	5.3	ng	216191	4	11.410	814545	20.0
5-Eicosene, (E)-	13.892	5.9	ng	291462	5	14.051	987170	20.0
Nonadecane	15.174	3.9	ng	125384	6	15.527	641772	20.0
Heneicosane	16.015	2.8	ng	89541	6	15.527	641772	20.0