

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
 Data File : BF139947.D
 Acq On : 23 Oct 2024 00:11
 Operator : RC/JU
 Sample : P4385-12
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-6

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: BF139947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	7	15	23	rBV	1719411	2773067	100.00%	12.777%
2	5.110	505	513	520	rVB	137148	201921	7.28%	0.930%
3	5.504	574	580	585	rBV	1913105	2487515	89.70%	11.461%
4	6.504	744	750	756	rBV	1769366	2343231	84.50%	10.797%
5	6.892	811	816	821	rBV	558445	695181	25.07%	3.203%
6	7.445	904	910	915	rBV	1190318	1525922	55.03%	7.031%
7	7.698	949	953	958	rBV	58372	70625	2.55%	0.325%
8	8.169	1028	1033	1038	rBV	644941	794376	28.65%	3.660%
9	8.381	1064	1069	1077	rVB2	24662	34424	1.24%	0.159%
10	9.245	1210	1216	1221	rBV	1973421	2420207	87.28%	11.151%
11	9.927	1326	1332	1337	rBV	567642	728930	26.29%	3.359%
12	10.639	1448	1453	1460	rVB	103851	134819	4.86%	0.621%
13	10.710	1460	1465	1479	rBV	1035550	1302897	46.98%	6.003%
14	11.410	1579	1584	1591	rBV	599716	749053	27.01%	3.451%
15	11.633	1617	1622	1631	rBV2	29582	46050	1.66%	0.212%
16	11.933	1664	1673	1686	rBV	218550	354945	12.80%	1.635%
17	12.192	1712	1717	1722	rBV2	27979	37340	1.35%	0.172%
18	12.621	1785	1790	1794	rBV	37856	56690	2.04%	0.261%
19	12.716	1802	1806	1813	rBV3	30969	52449	1.89%	0.242%
20	12.816	1819	1823	1826	rBV	31636	42222	1.52%	0.195%
21	12.851	1826	1829	1834	rVB	29780	40352	1.46%	0.186%
22	12.998	1848	1854	1859	rBV	2099802	2677617	96.56%	12.337%
23	13.521	1940	1943	1947	rBV	23573	30993	1.12%	0.143%
24	13.892	2001	2006	2015	rBV	224800	349135	12.59%	1.609%
25	14.051	2027	2033	2043	rBV	642691	888194	32.03%	4.092%
26	14.521	2110	2113	2118	rBV2	49682	66894	2.41%	0.308%
27	14.910	2176	2179	2186	rVB	54625	76028	2.74%	0.350%
28	15.174	2221	2224	2228	rBV	38368	61849	2.23%	0.285%
29	15.527	2279	2284	2297	rVB	362741	592492	21.37%	2.730%
30	16.015	2363	2367	2371	rVB	45707	68009	2.45%	0.313%

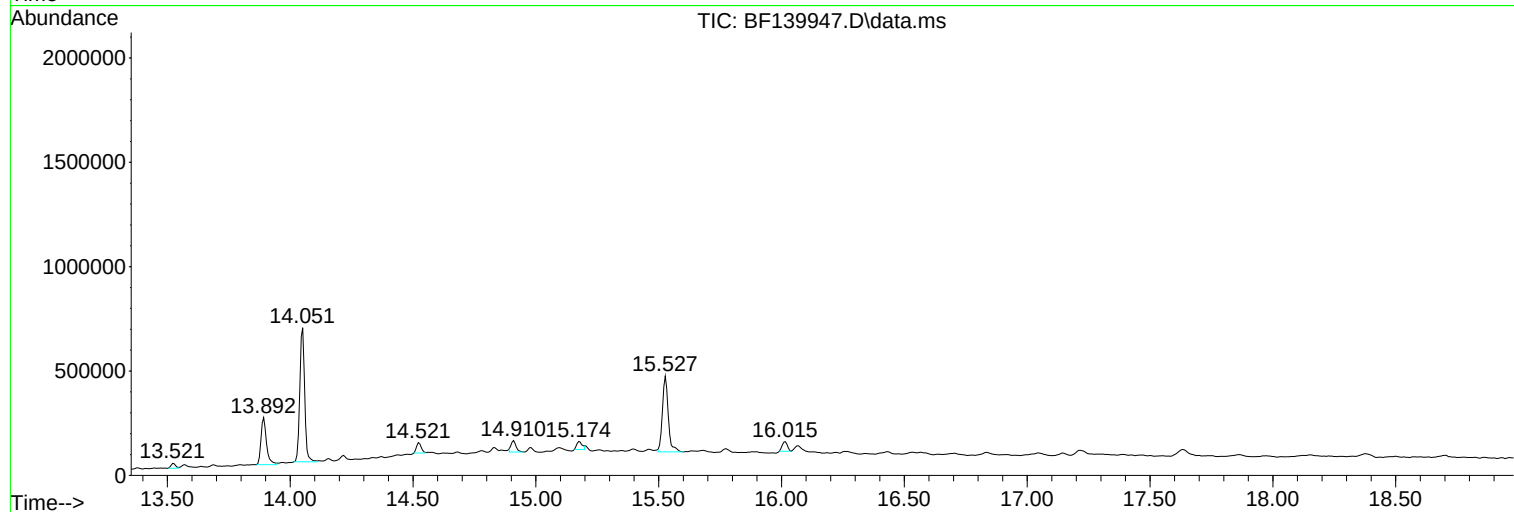
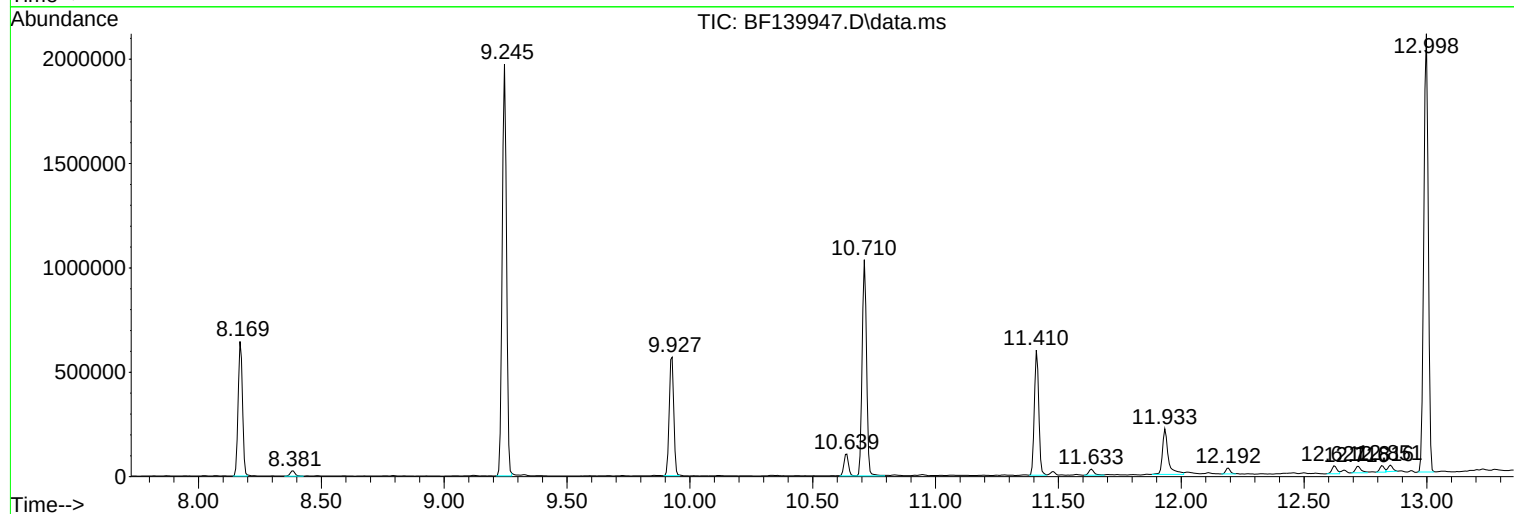
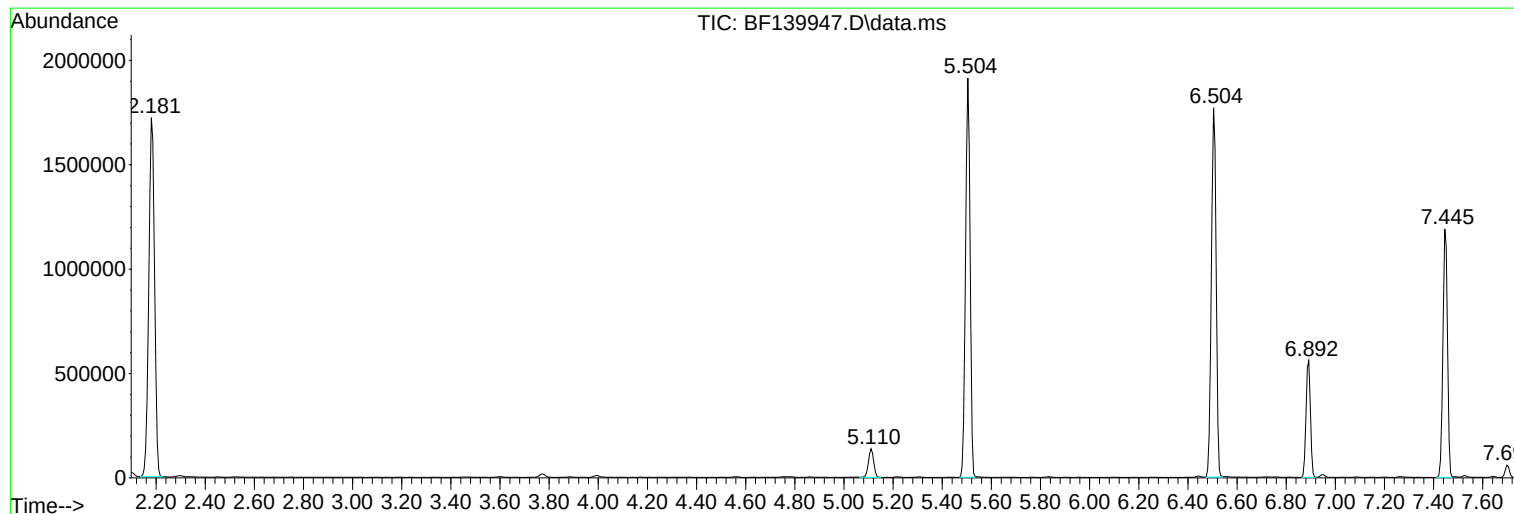
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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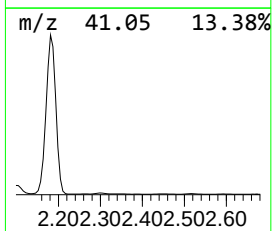
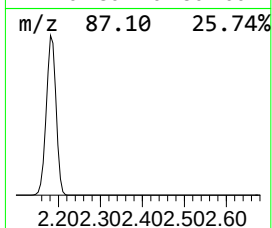
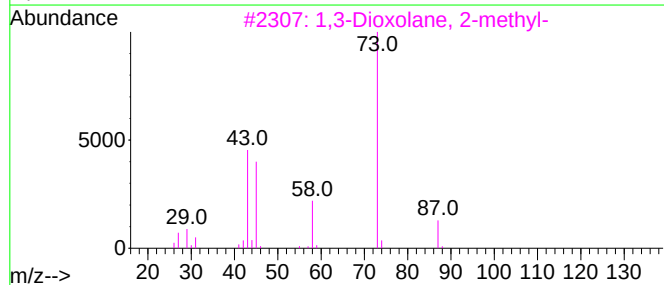
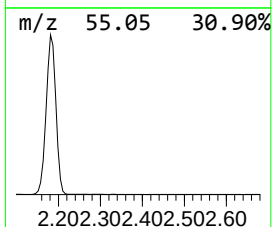
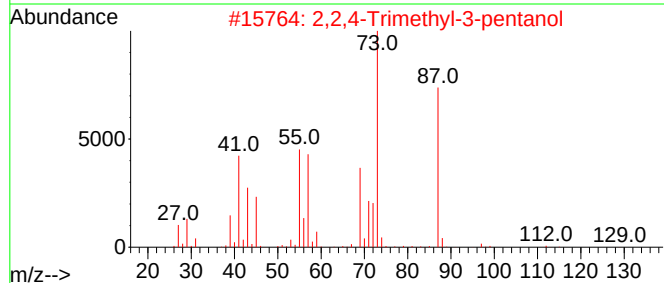
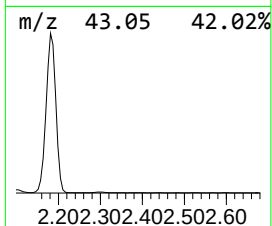
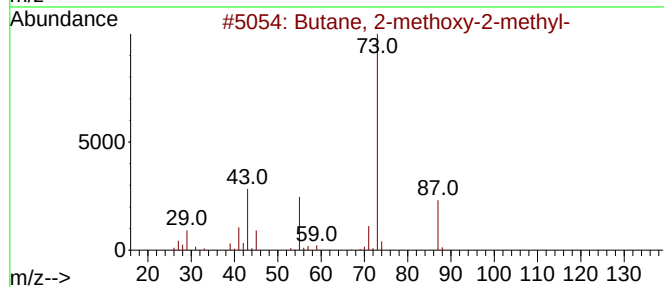
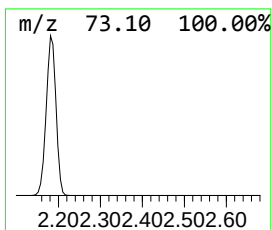
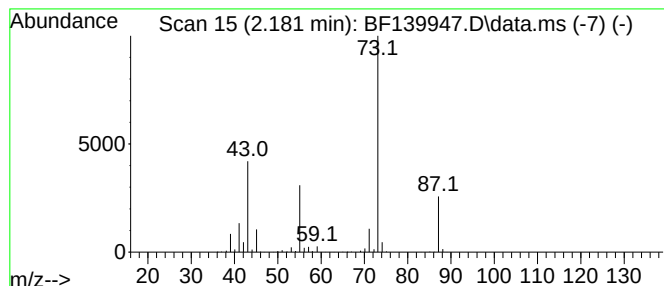
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.181	79.78 ng	2773070	1,4-Dichlorobenzene-d4	6.892

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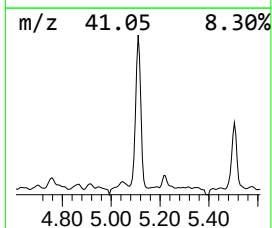
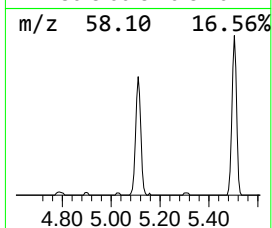
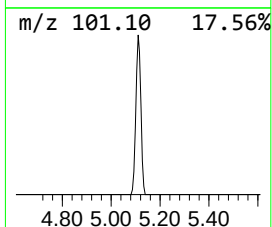
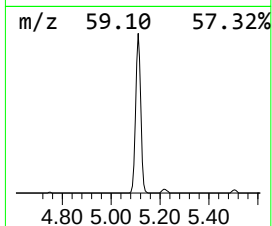
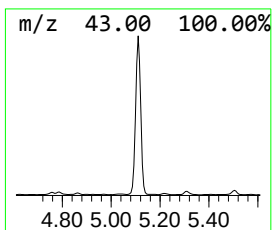
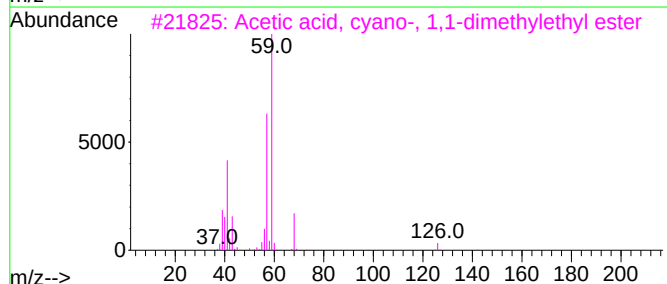
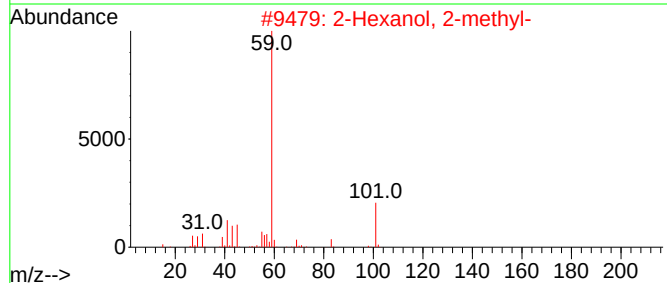
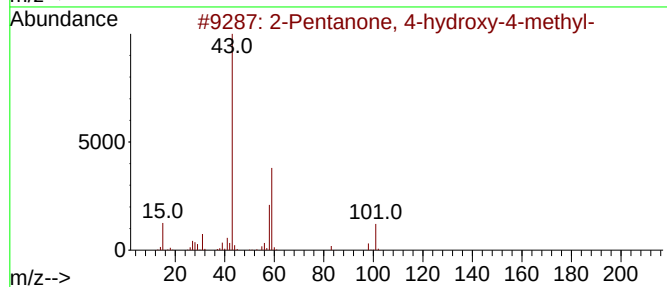
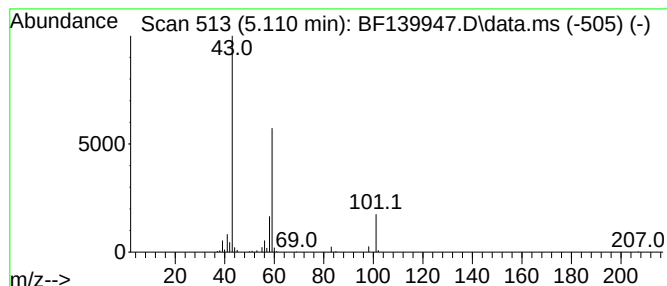
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.81 ng	201921	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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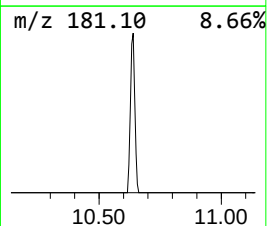
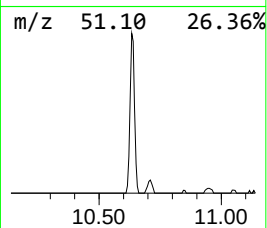
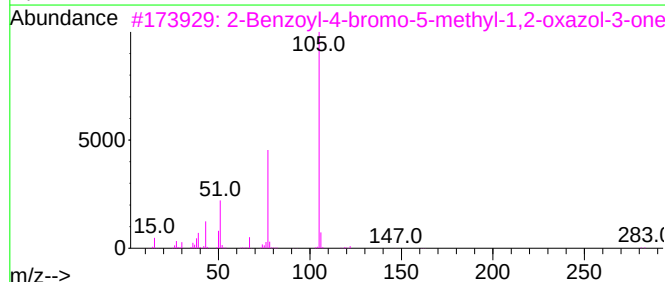
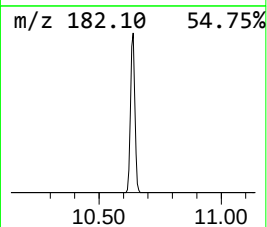
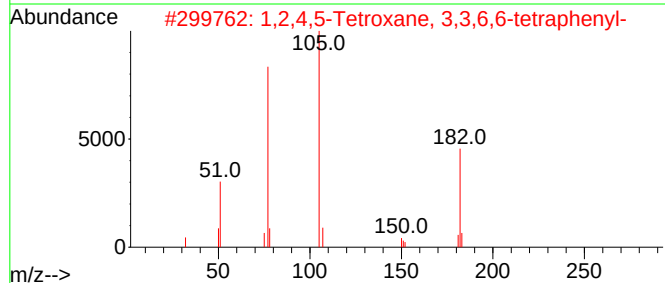
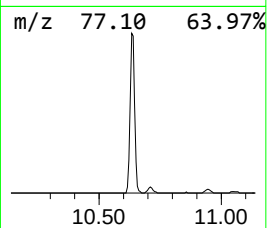
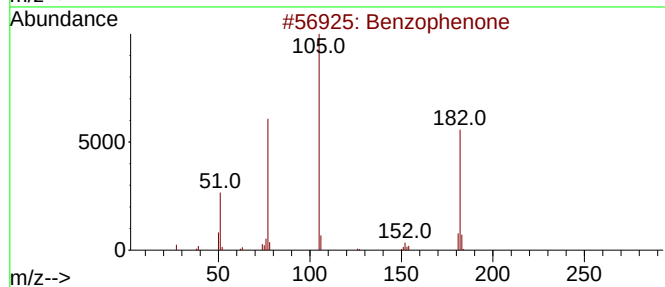
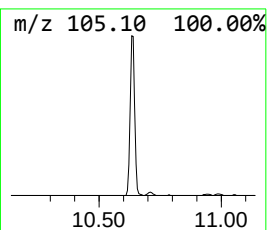
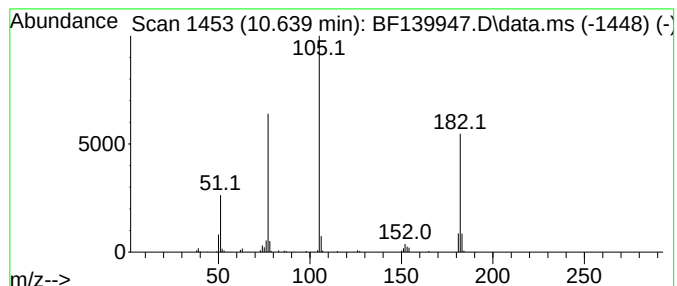
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	3.70 ng	134819	Acenaphthene-d10	9.927

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47



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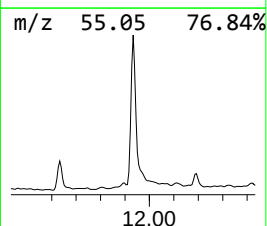
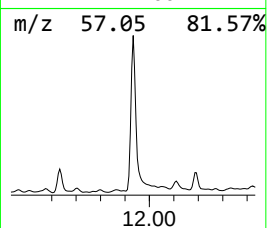
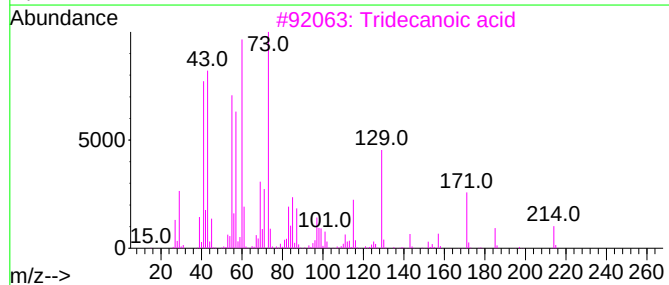
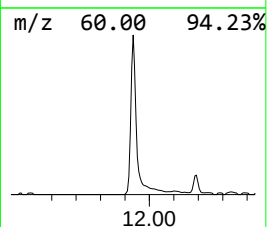
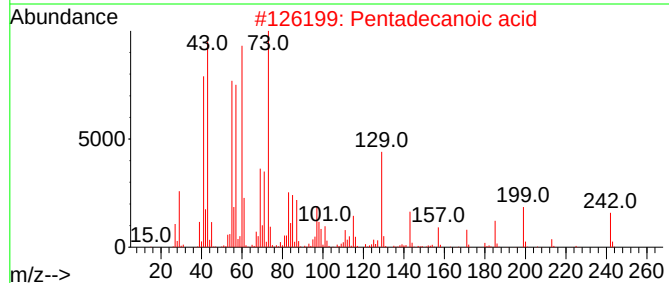
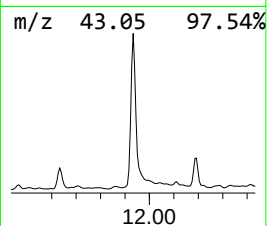
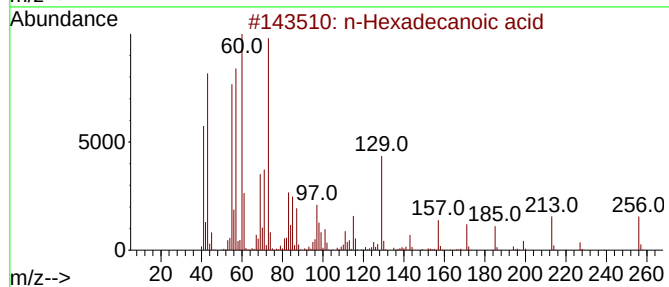
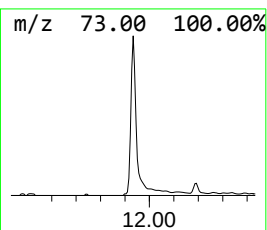
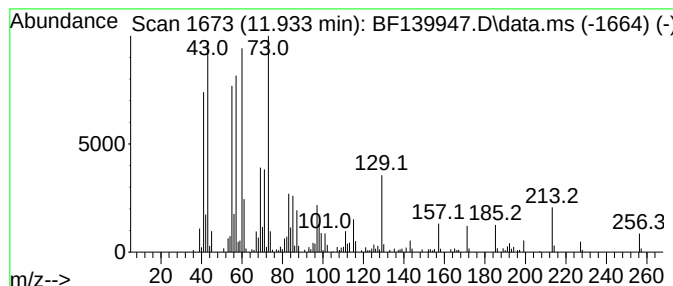
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.933	9.48 ng	354945	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
3	Tridecanoic acid		214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
5	Octanoic acid		144	C8H16O2	000124-07-2	46



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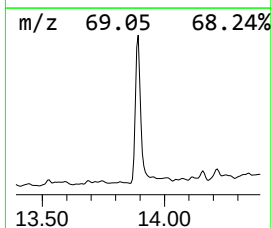
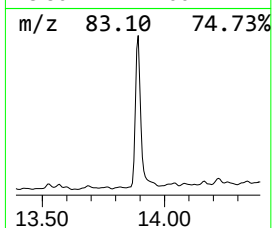
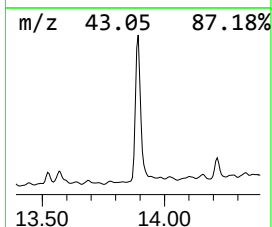
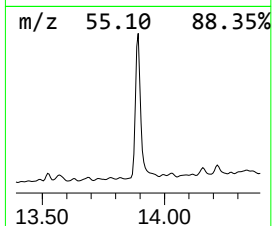
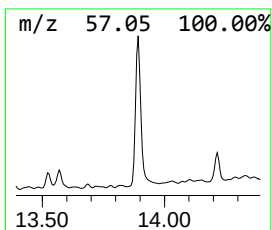
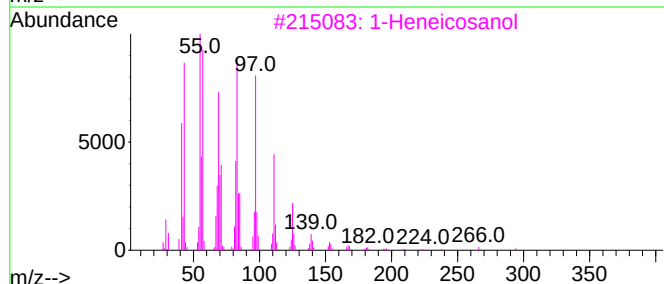
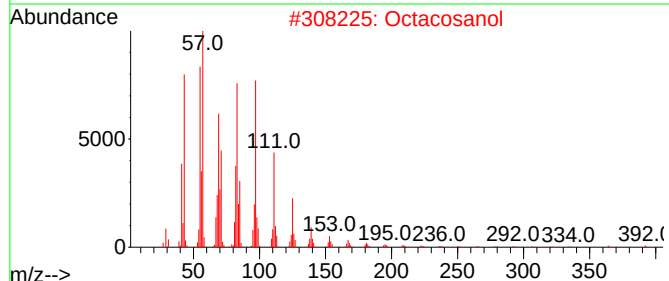
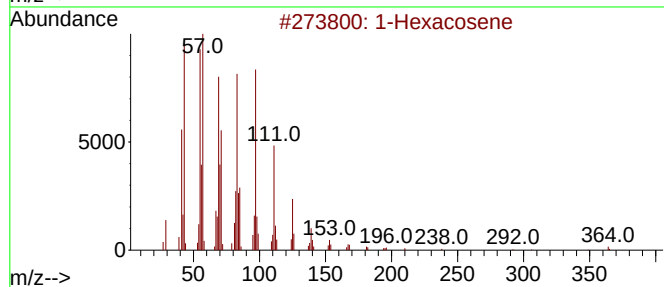
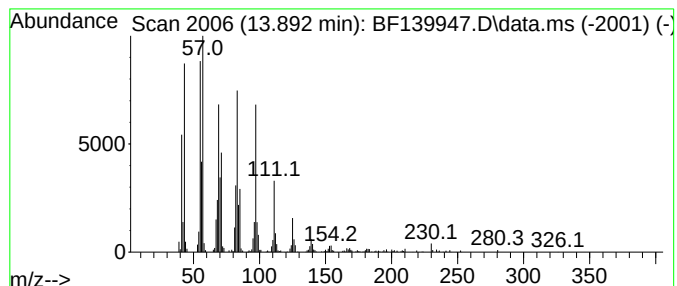
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	7.86 ng	349135	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosene	364	C26H52	018835-33-1	94
2			Octacosanol	410	C28H58O	000557-61-9	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Cyclopentadecane	210	C15H30	000295-48-7	93
5			1-Docosene	308	C22H44	001599-67-3	91



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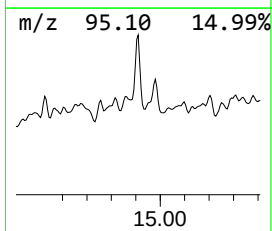
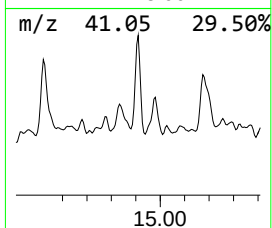
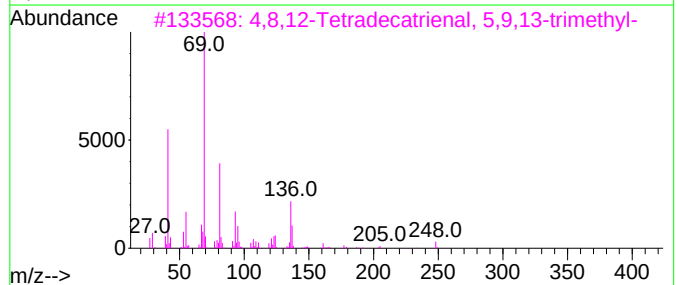
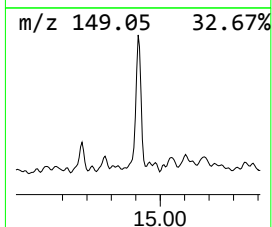
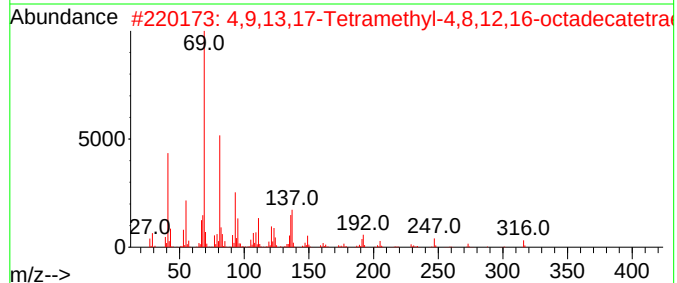
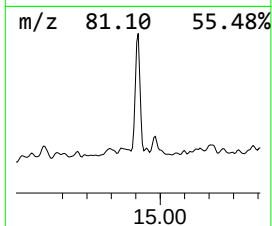
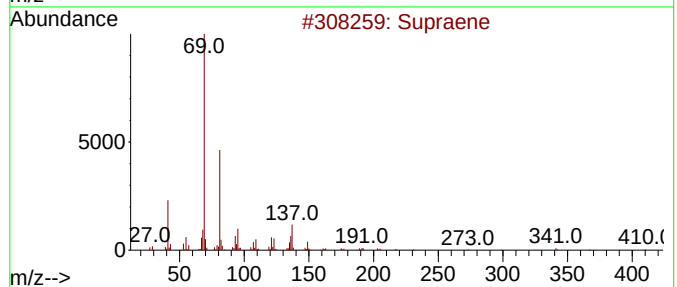
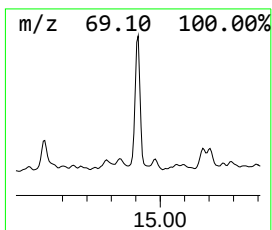
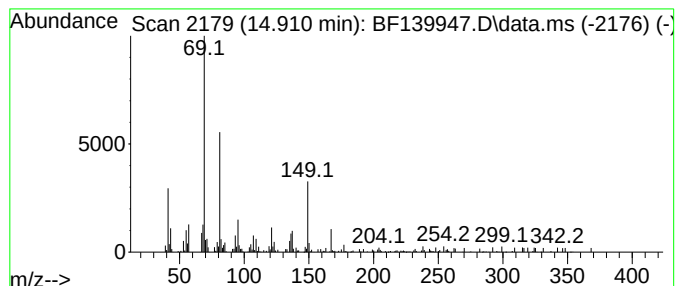
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	2.57 ng	76028	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	62
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	62
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	58
4			Umbelliprenin	366	C24H30O3	023838-17-7	53
5			(3E,7E)-4,8,12-Trimethyltrideca-...	218	C16H26	062235-06-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139947.D
Acq On : 23 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-6

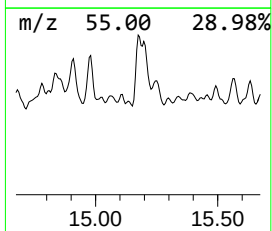
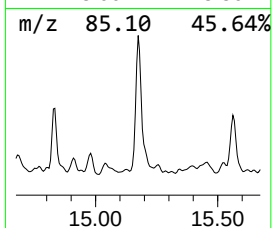
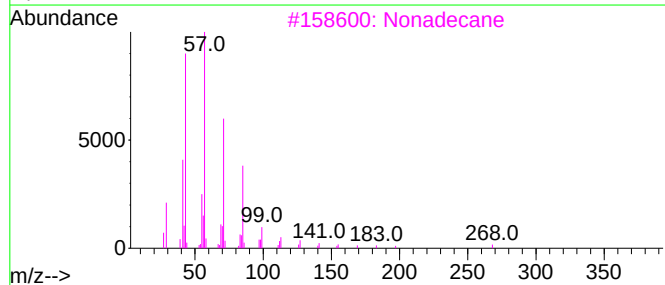
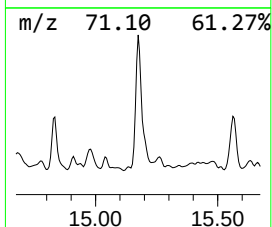
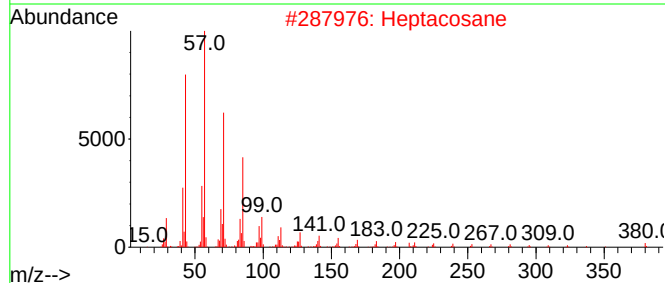
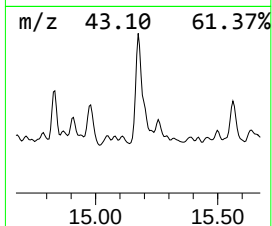
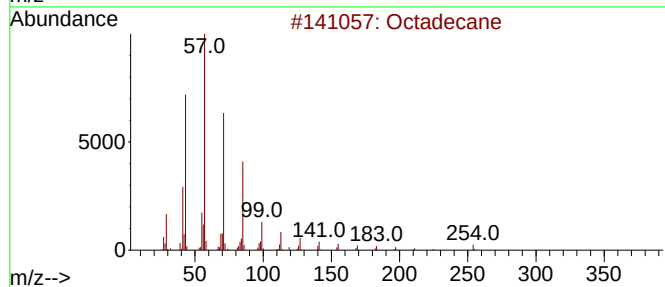
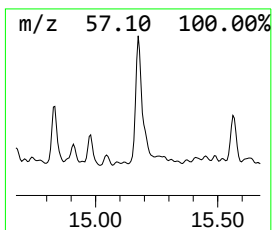
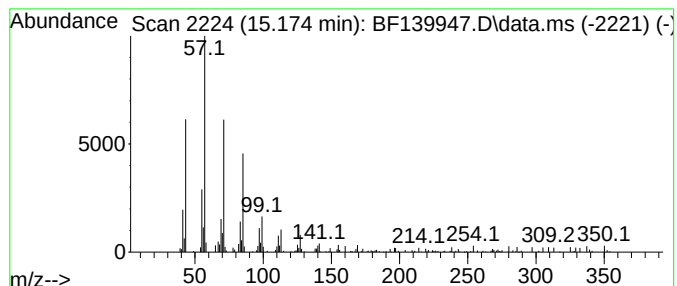
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.09 ng	61849	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	97
2			Heptacosane	380	C27H56	000593-49-7	90
3			Nonadecane	268	C19H40	000629-92-5	90
4			Octacosane	394	C28H58	000630-02-4	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139947.D
Acq On : 23 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

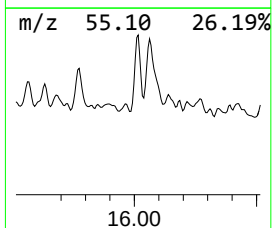
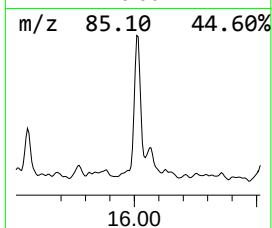
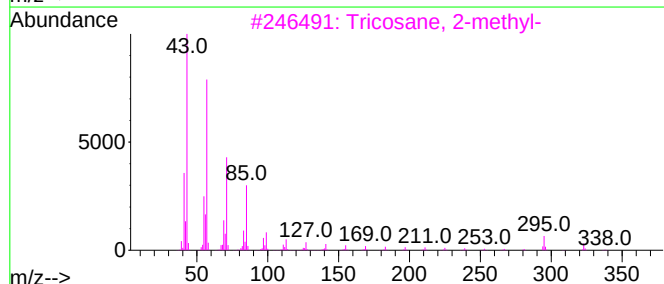
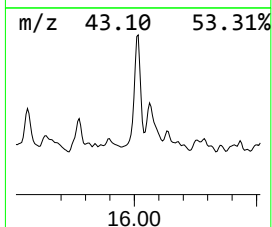
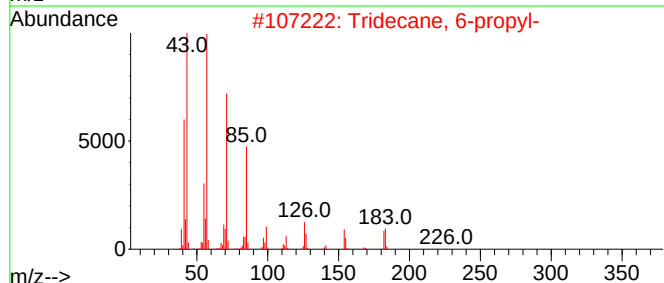
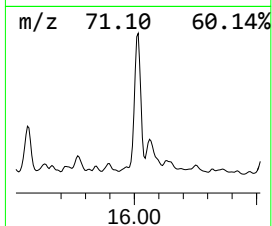
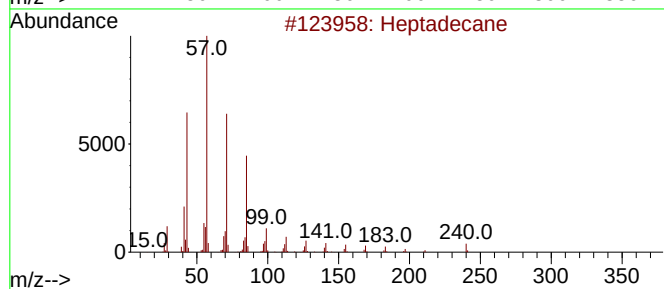
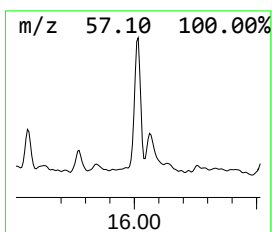
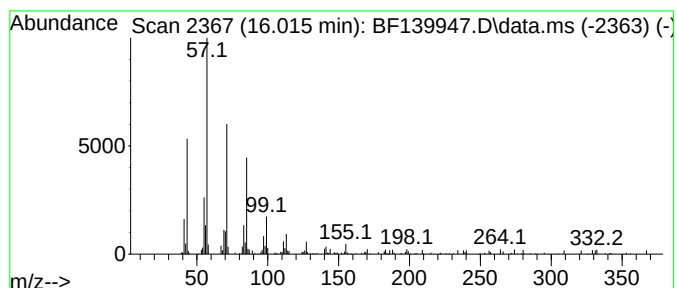
Instrument :
BNA_F
ClientSampleId :
SP-6

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 8 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.015	2.30 ng	68009	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Tridecane, 6-propyl-	226	C16H34	055045-10-8	93
3	Tricosane, 2-methyl-	338	C24H50	001928-30-9	90
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
5	Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102224\
Data File : BF139947.D
Acq On : 23 Oct 2024 00:11
Operator : RC/JU
Sample : P4385-12
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-6

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.181	79.8	ng	2773070	1	6.892	695181	20.0
2-Pentanone, 4-...	5.110	5.8	ng	201921	1	6.892	695181	20.0
Benzophenone	10.639	3.7	ng	134819	3	9.927	728930	20.0
n-Hexadecanoic ...	11.933	9.5	ng	354945	4	11.410	749053	20.0
1-Hexacosene	13.892	7.9	ng	349135	5	14.051	888194	20.0
Supraene	14.910	2.6	ng	76028	6	15.527	592492	20.0
Octadecane	15.174	2.1	ng	61849	6	15.527	592492	20.0
Heptadecane	16.015	2.3	ng	68009	6	15.527	592492	20.0