

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
 Data File : BF124219.D
 Acq On : 9 Jun 2021 20:59
 Operator : JU/CG
 Sample : M2628-01 5X
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HD-02-060721

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124219.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.475	572	576	586	rBB	201533	184062	28.23%	3.517%
2	6.486	745	748	756	rBB	234297	193188	29.63%	3.691%
3	6.851	806	810	813	rBV	270327	235756	36.16%	4.504%
4	7.410	901	905	909	rBV	143522	129068	19.80%	2.466%
5	8.133	1024	1028	1031	rVB	387666	291399	44.70%	5.568%
6	9.204	1207	1210	1214	rBV	309763	239052	36.67%	4.567%
7	9.286	1220	1224	1227	rBV2	15325	14563	2.23%	0.278%
8	9.322	1227	1230	1233	rBV2	18698	18123	2.78%	0.346%
9	9.598	1274	1277	1281	rBV2	48219	49464	7.59%	0.945%
10	9.751	1298	1303	1306	rBV4	4439	7566	1.16%	0.145%
11	9.816	1311	1314	1318	rVV	25969	23378	3.59%	0.447%
12	9.886	1322	1326	1330	rVB	399224	318669	48.88%	6.089%
13	10.057	1349	1355	1356	rBV6	5540	9758	1.50%	0.186%
14	10.139	1365	1369	1373	rBV2	9870	12354	1.89%	0.236%
15	10.316	1394	1399	1402	rBB	37809	28792	4.42%	0.550%
16	10.533	1432	1436	1441	rBV2	19881	26533	4.07%	0.507%
17	10.674	1457	1460	1465	rVB	136954	115831	17.77%	2.213%
18	10.751	1471	1473	1477	rBV4	6985	10247	1.57%	0.196%
19	10.786	1477	1479	1484	rVV3	47269	60629	9.30%	1.158%
20	11.239	1552	1556	1558	rBV2	35842	34683	5.32%	0.663%
21	11.268	1558	1561	1567	rVB3	21332	23214	3.56%	0.444%
22	11.374	1576	1579	1582	rBV	352512	271009	41.57%	5.178%
23	11.398	1582	1583	1587	rVB	20744	12085	1.85%	0.231%
24	11.551	1606	1609	1611	rBV4	6724	7908	1.21%	0.151%
25	11.616	1616	1620	1623	rBV5	8302	10048	1.54%	0.192%
26	11.663	1625	1628	1630	rVV	33851	25246	3.87%	0.482%
27	11.686	1630	1632	1634	rVB2	14330	10425	1.60%	0.199%
28	11.763	1641	1645	1648	rBV	288507	213674	32.77%	4.082%
29	11.898	1666	1668	1671	rBV2	37334	33917	5.20%	0.648%
30	11.986	1679	1683	1685	rBV3	14048	15274	2.34%	0.292%
31	12.010	1685	1687	1691	rVB3	10932	11525	1.77%	0.220%
32	12.068	1694	1697	1702	rVB2	24679	20903	3.21%	0.399%
33	12.174	1711	1715	1716	rBV4	8972	9340	1.43%	0.178%
34	12.427	1755	1758	1759	rBV3	18067	20192	3.10%	0.386%
35	12.451	1759	1762	1764	rVV	734646	651971	100.00%	12.457%
36	12.474	1764	1766	1773	rVB	734465	641707	98.43%	12.261%

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Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	12.527	1773	1775	1776	rVB2	11963	7363	1.13%	0.141%
38	12.557	1776	1780	1783	rBV	130453	109499	16.80%	2.092%
39	12.586	1783	1785	1788	rBV	49358	51685	7.93%	0.988%
40	12.686	1799	1802	1807	rVB6	19762	25104	3.85%	0.480%
41	12.792	1818	1820	1821	rBV2	17233	14840	2.28%	0.284%
42	12.821	1822	1825	1832	rVV2	50917	75554	11.59%	1.444%
43	12.880	1832	1835	1837	rVB4	20109	20075	3.08%	0.384%
44	12.957	1842	1848	1851	rBV	263543	222764	34.17%	4.256%
45	13.039	1858	1862	1866	rBV7	13848	27729	4.25%	0.530%
46	13.115	1873	1875	1877	rBV3	27811	21647	3.32%	0.414%
47	13.139	1877	1879	1884	rVB6	17744	21946	3.37%	0.419%
48	13.192	1885	1888	1889	rBV2	22448	23289	3.57%	0.445%
49	13.257	1896	1899	1900	rBV3	15040	16431	2.52%	0.314%
50	13.280	1901	1903	1906	rVB3	18966	14604	2.24%	0.279%
51	13.345	1912	1914	1916	rBV3	15981	11519	1.77%	0.220%
52	13.498	1938	1940	1941	rBV2	12789	8194	1.26%	0.157%
53	13.527	1943	1945	1947	rBV3	14897	12755	1.96%	0.244%
54	13.751	1981	1983	1984	rBV2	15359	8571	1.31%	0.164%
55	14.015	2025	2028	2032	rBV	277040	265255	40.69%	5.068%
56	14.280	2071	2073	2074	rBV2	20212	15451	2.37%	0.295%
57	15.498	2277	2280	2290	rVB2	139094	226327	34.71%	4.324%
58	16.856	2510	2511	2514	rBV3	17644	14912	2.29%	0.285%
59	17.427	2606	2608	2612	rVB5	19917	20258	3.11%	0.387%
60	17.662	2644	2648	2649	rBV4	14888	16582	2.54%	0.317%

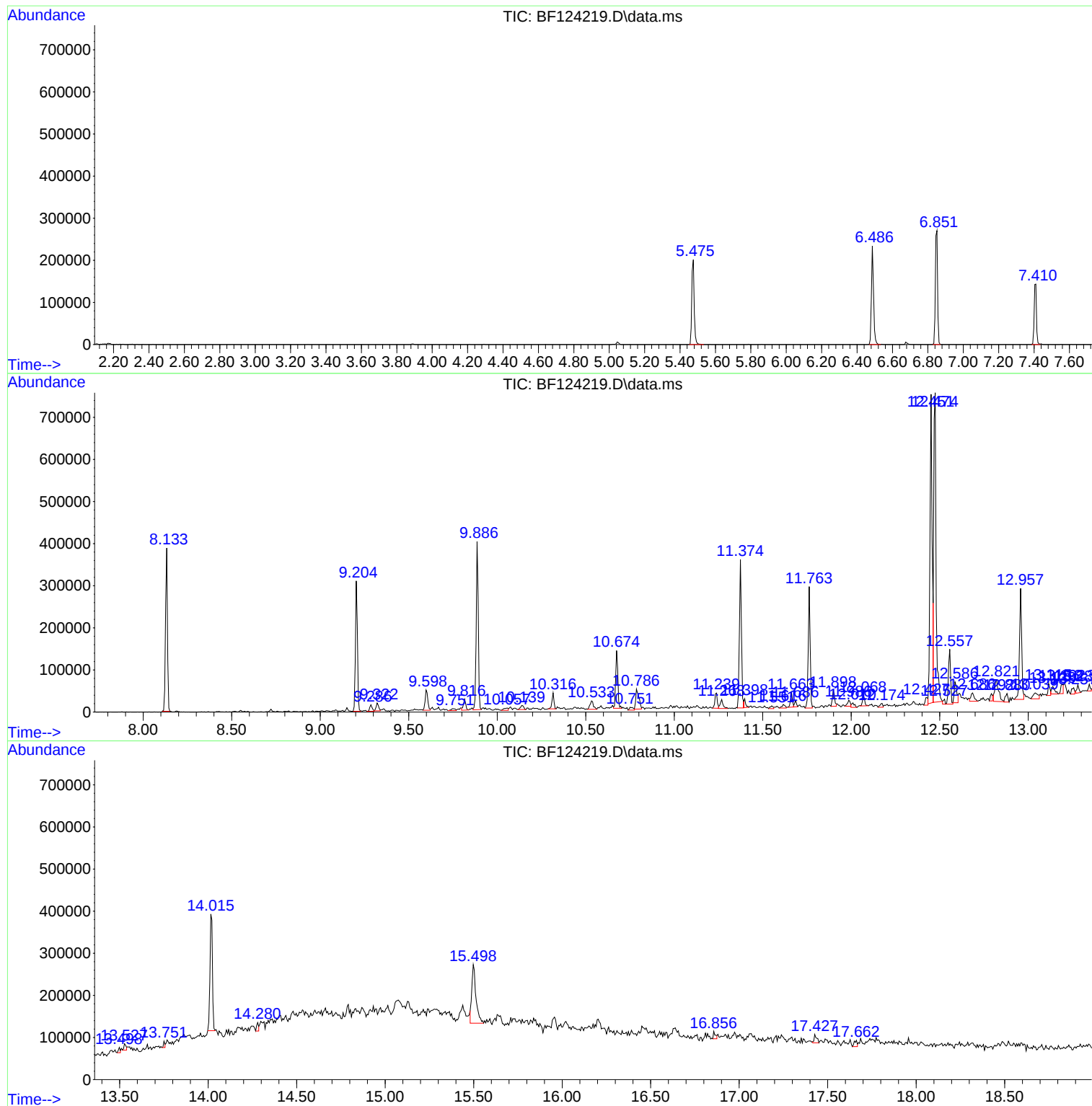
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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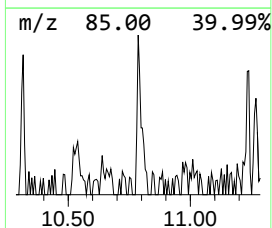
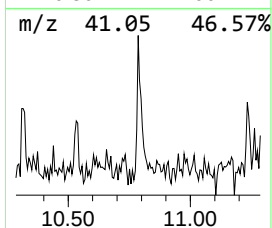
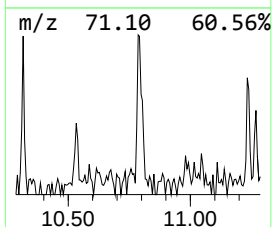
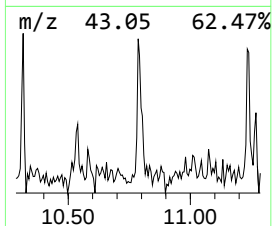
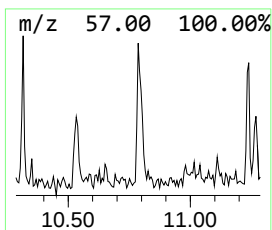
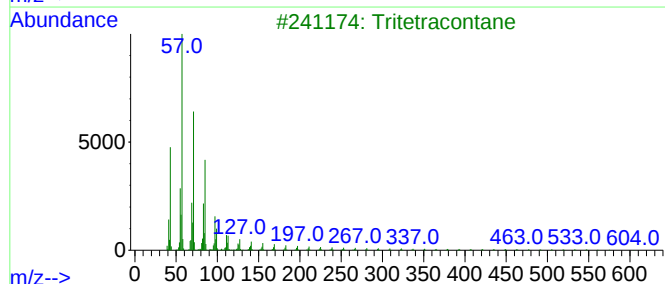
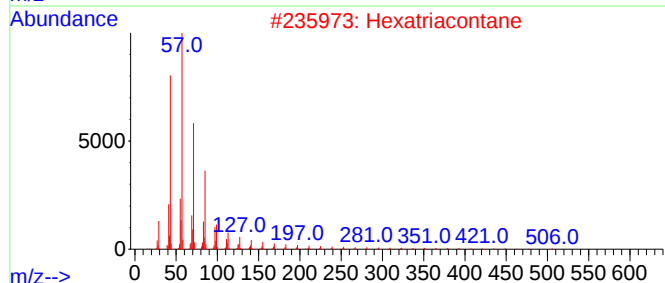
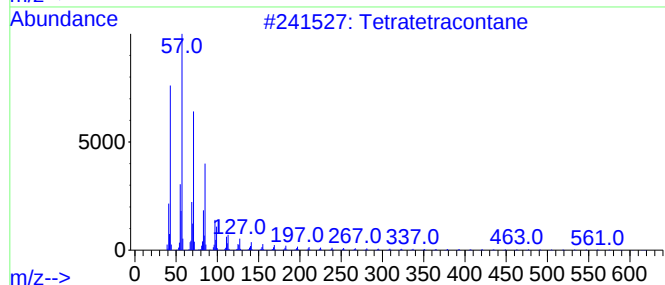
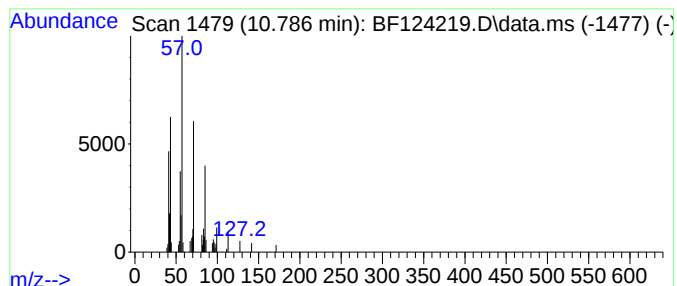
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.786	4.47 ng	60629	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	86
2			Hexatriacontane	507	C36H74	000630-06-8	78
3			Tritetracontane	605	C43H88	007098-21-7	78
4			Heneicosane	296	C21H44	000629-94-7	78
5			Octadecane	254	C18H38	000593-45-3	78



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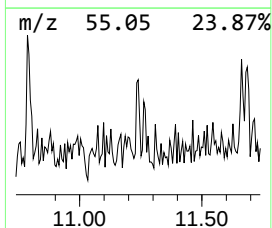
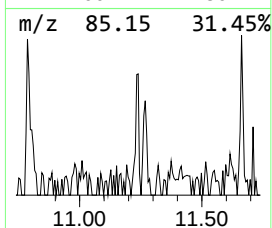
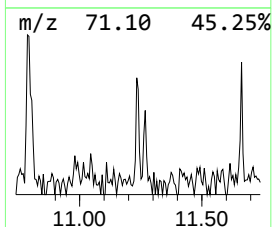
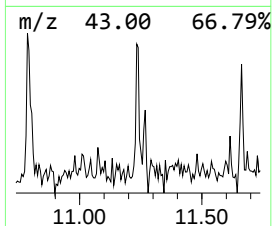
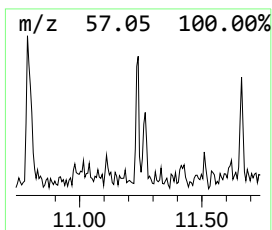
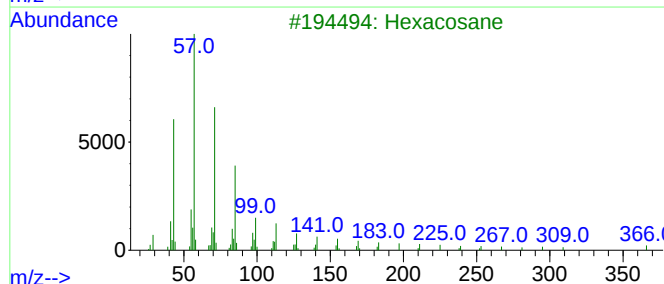
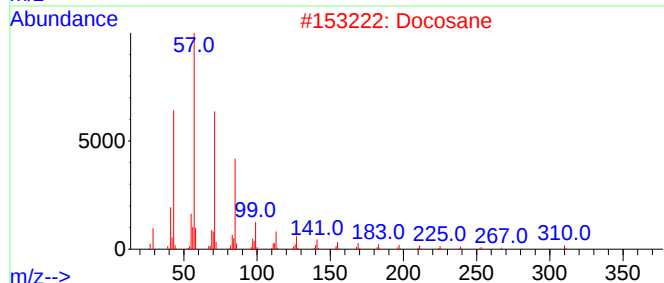
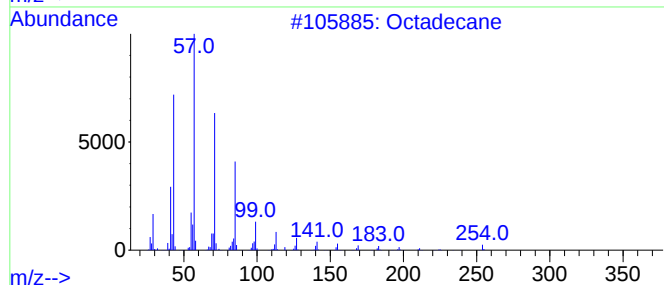
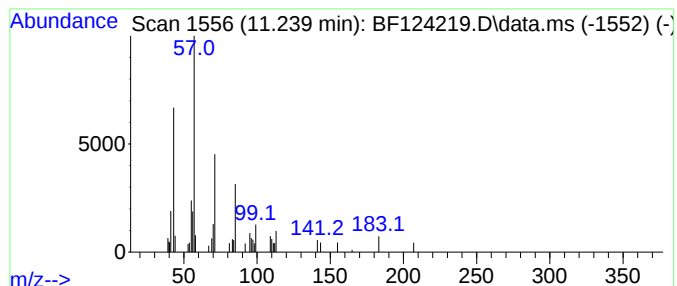
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.239	2.56 ng	34683	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	78
2			Docosane	310	C22H46	000629-97-0	78
3			Hexacosane	366	C26H54	000630-01-3	72
4			Pentacosane	352	C25H52	000629-99-2	72
5			Octacosane	394	C28H58	000630-02-4	72



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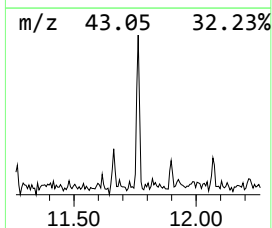
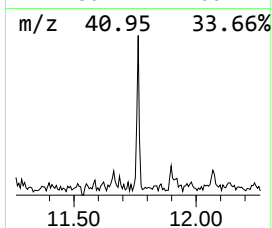
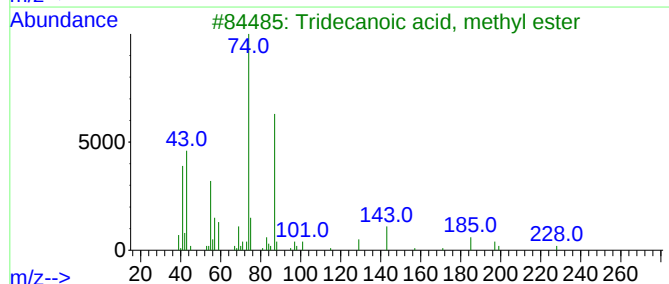
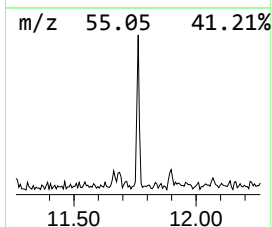
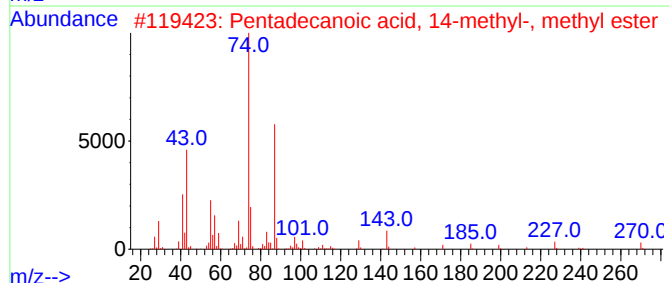
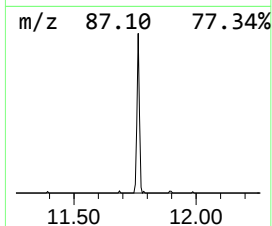
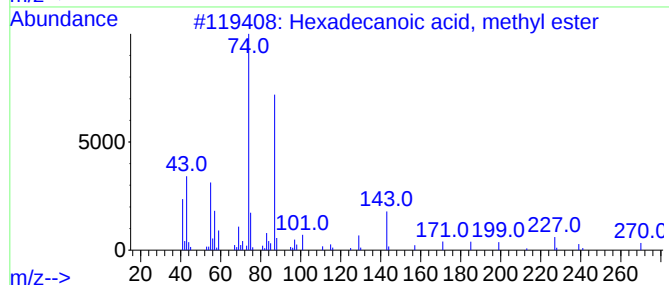
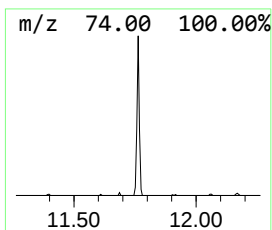
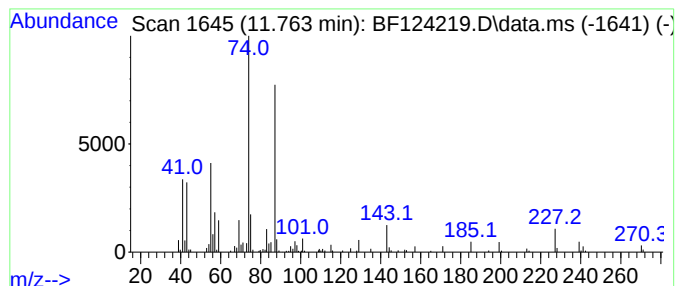
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.763	15.77 ng	213674	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	96
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	90
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87



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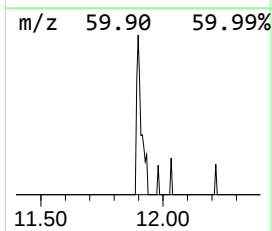
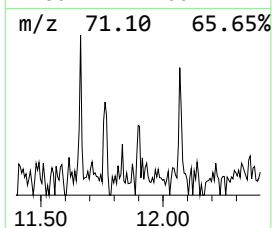
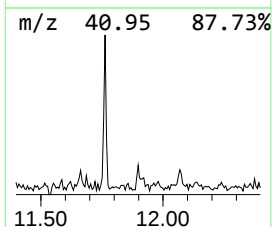
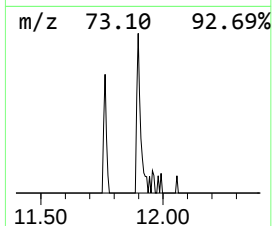
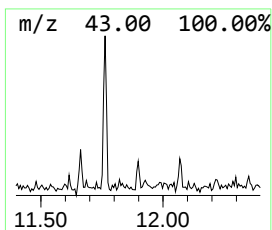
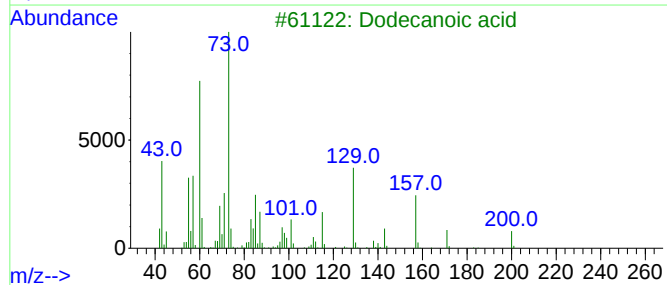
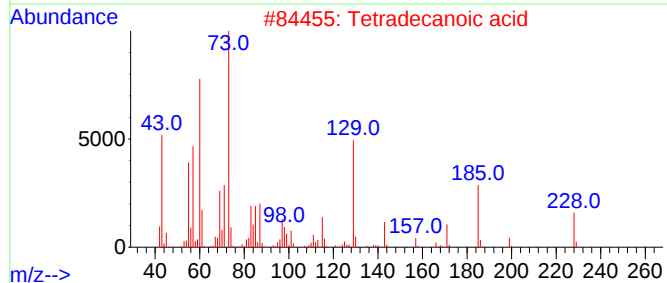
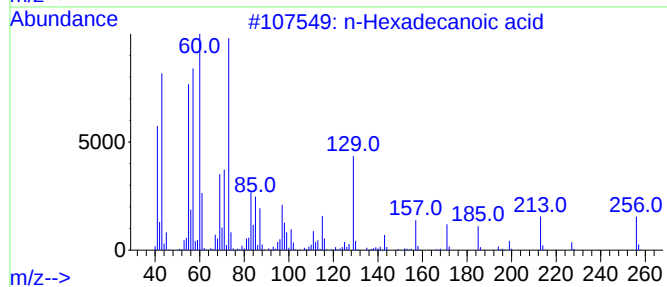
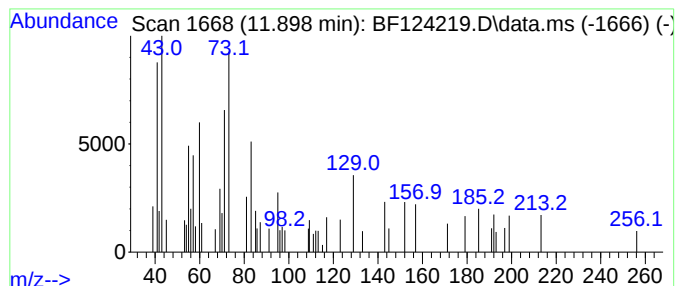
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	2.50 ng	33917	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
3			Dodecanoic acid	200	C12H24O2	000143-07-7	43
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	38
5			Tridecanoic acid	214	C13H26O2	000638-53-9	27



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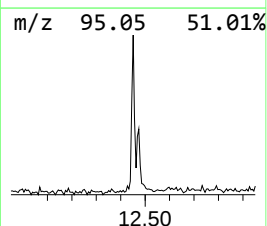
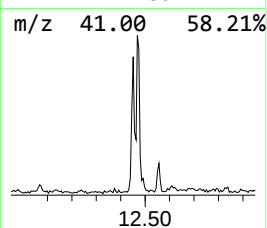
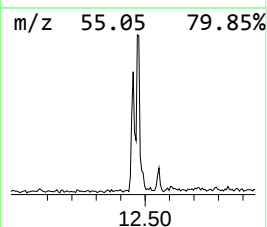
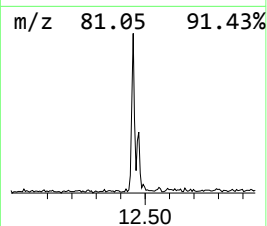
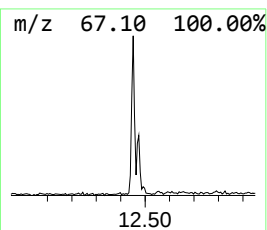
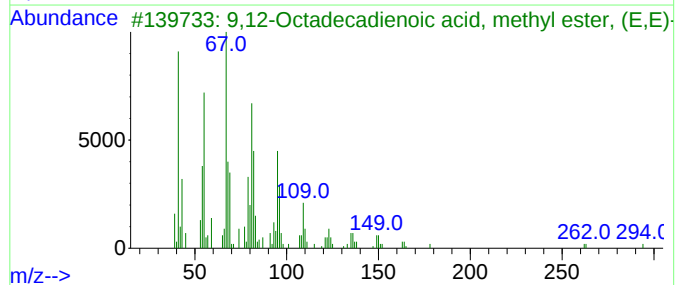
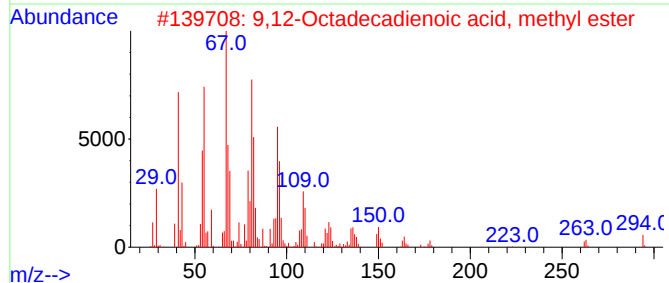
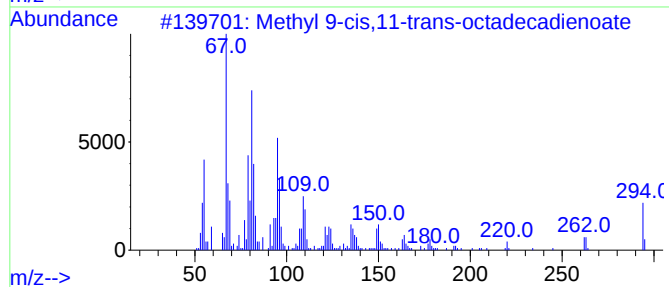
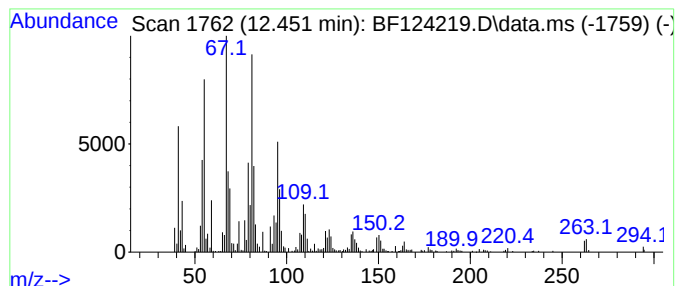
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	48.11 ng	651971	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
2			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
4			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98
5			8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	97



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124219.D
Acq On : 9 Jun 2021 20:59
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

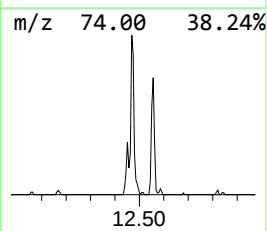
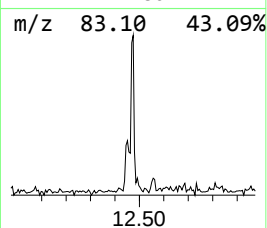
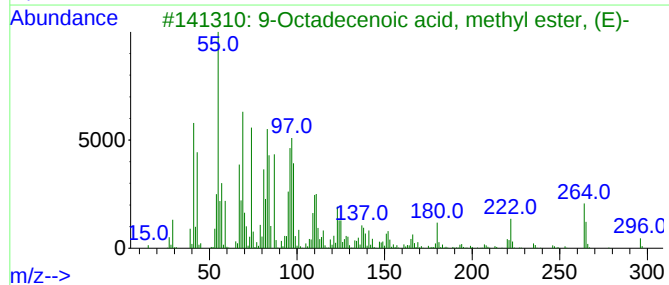
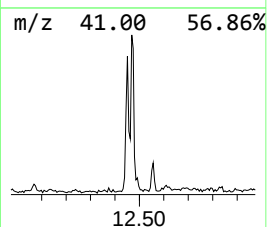
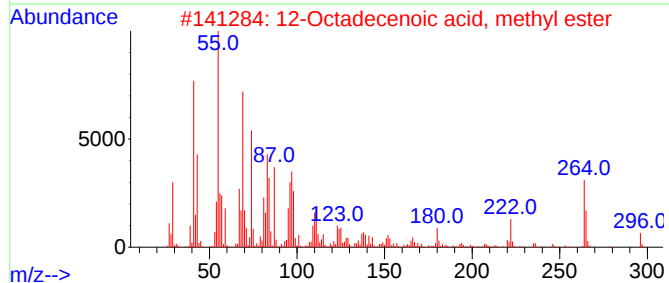
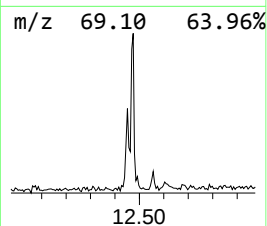
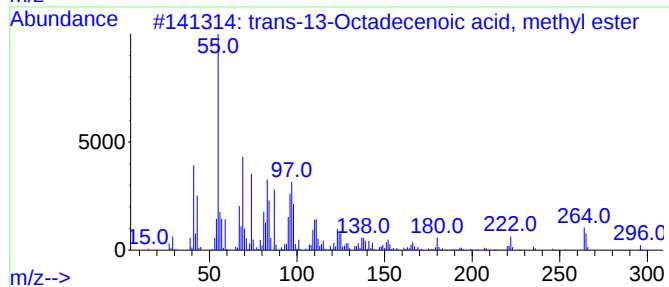
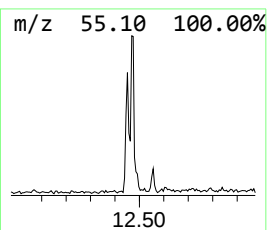
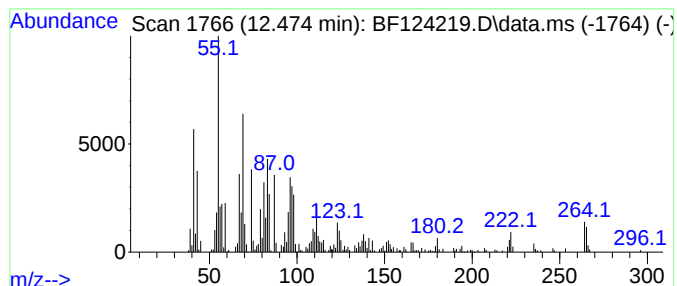
Instrument :
BNA_F
ClientSampleId :
HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 trans-13-Octadecenoic acid,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.474	47.36 ng	641707	Phenanthrene-d10	11.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	91
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91
4	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	80
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124219.D
Acq On : 9 Jun 2021 20:59
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-060721

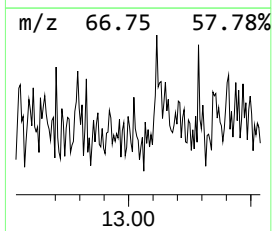
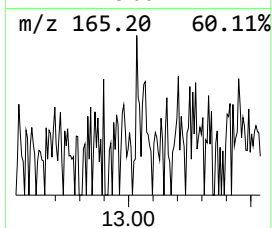
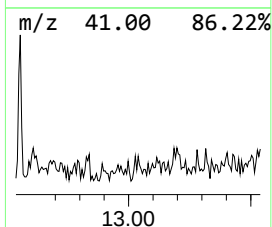
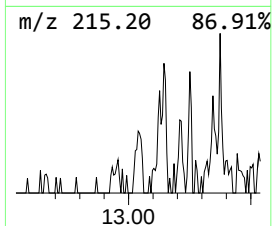
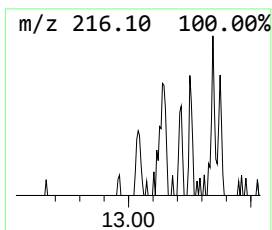
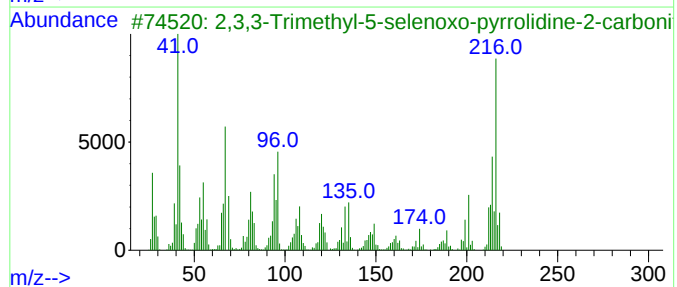
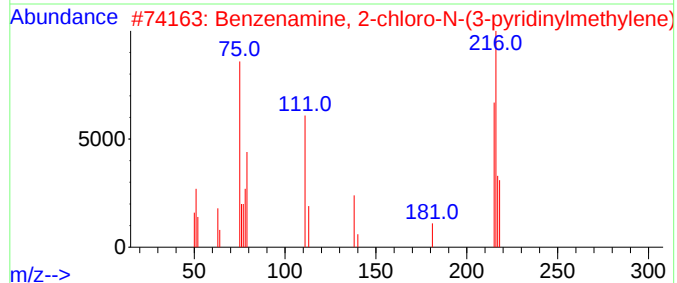
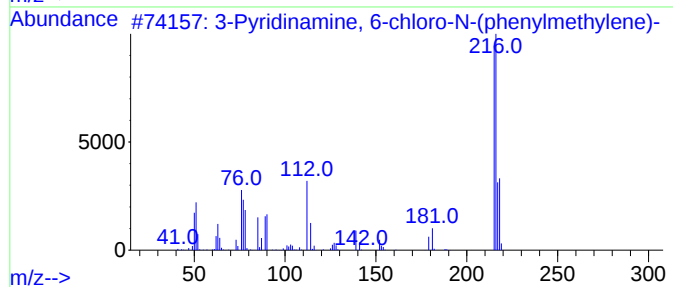
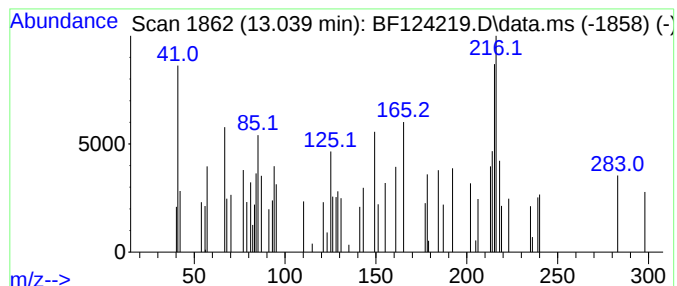
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown13.039 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.039	2.09 ng	27729	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pyridinamine, 6-chloro-N-(phen...	216	C12H9ClN2	005325-71-3	32		
2	Benzenamine, 2-chloro-N-(3-pyrid...	216	C12H9ClN2	041855-59-8	32		
3	2,3,3-Trimethyl-5-selenoxo-pyrro...	216	C8H12N2Se	1000185-26-0	27		
4	trans-p-(Trifluoromethyl)cinnami...	216	C10H7F3O2	016642-92-5	16		
5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	16		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124219.D
Acq On : 9 Jun 2021 20:59
Operator : JU/CG
Sample : M2628-01 5X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-02-060721

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tetratetracontane	10.786	4.5	ng	60629	4	11.374	271009	20.0
Octadecane	11.239	2.6	ng	34683	4	11.374	271009	20.0
Hexadecanoic ac...	11.763	15.8	ng	213674	4	11.374	271009	20.0
n-Hexadecanoic ...	11.898	2.5	ng	33917	4	11.374	271009	20.0
Methyl 9-cis,11...	12.451	48.1	ng	651971	4	11.374	271009	20.0
trans-13-Octade...	12.474	47.4	ng	641707	4	11.374	271009	20.0
unknown13.039	13.039	2.1	ng	27729	5	14.021	265255	20.0