

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
 Data File : BF126228.D
 Acq On : 17 Dec 2021 11:08
 Operator : JU/CG
 Sample : PB141306BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126228.D\data.ms

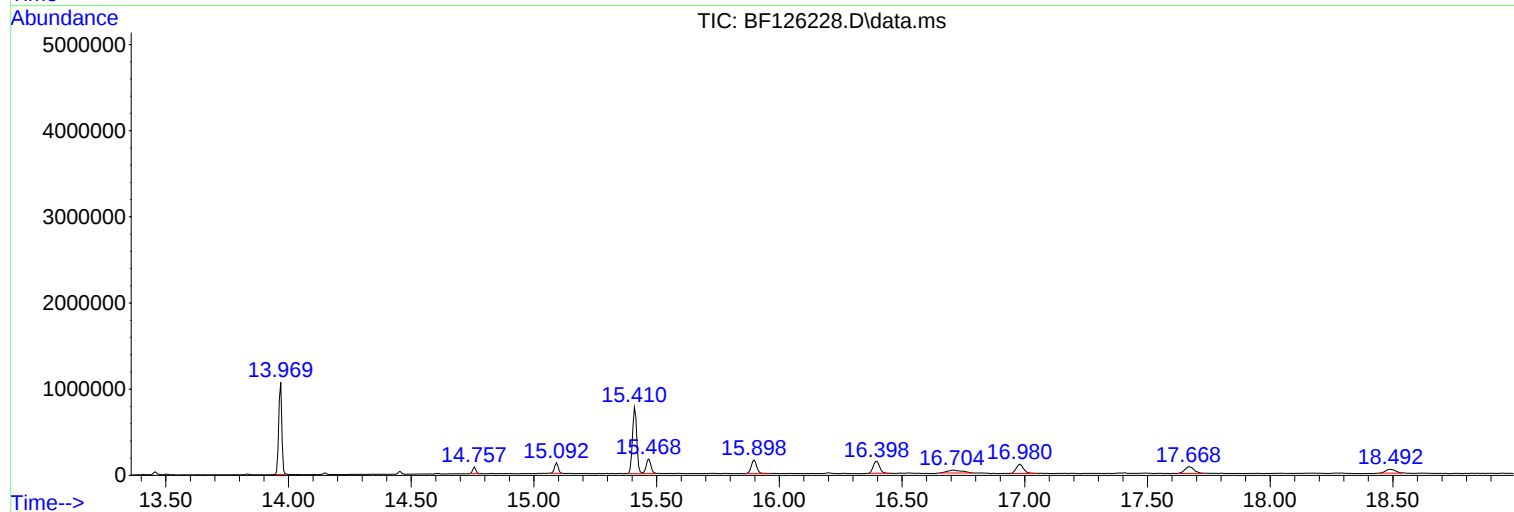
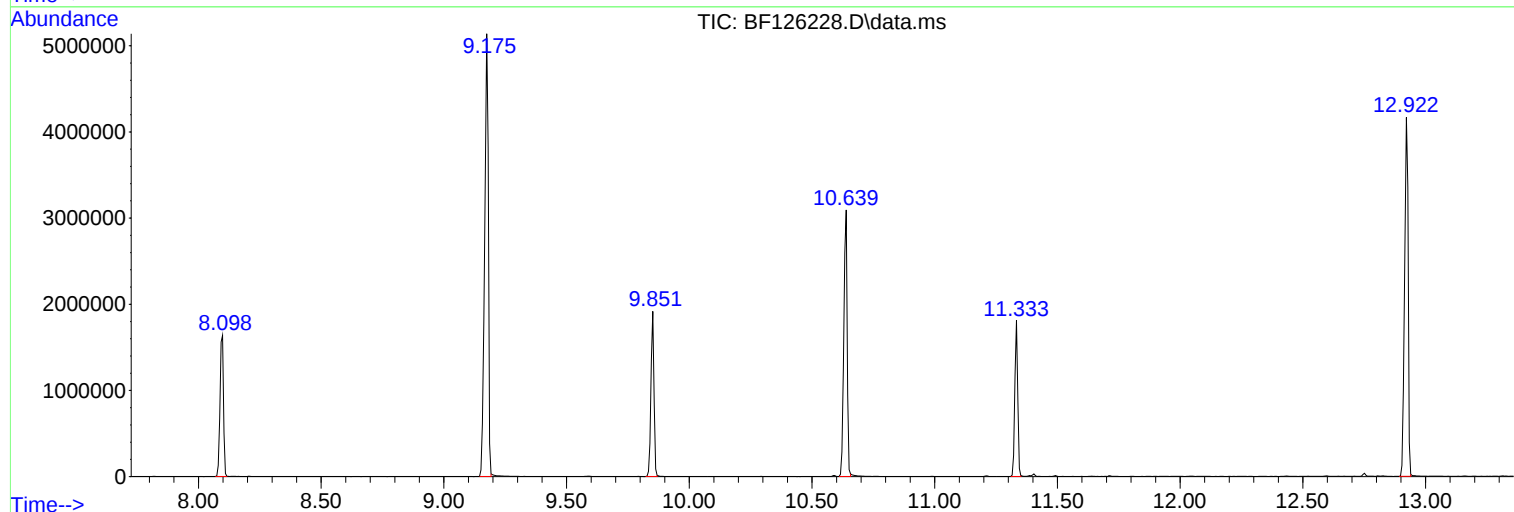
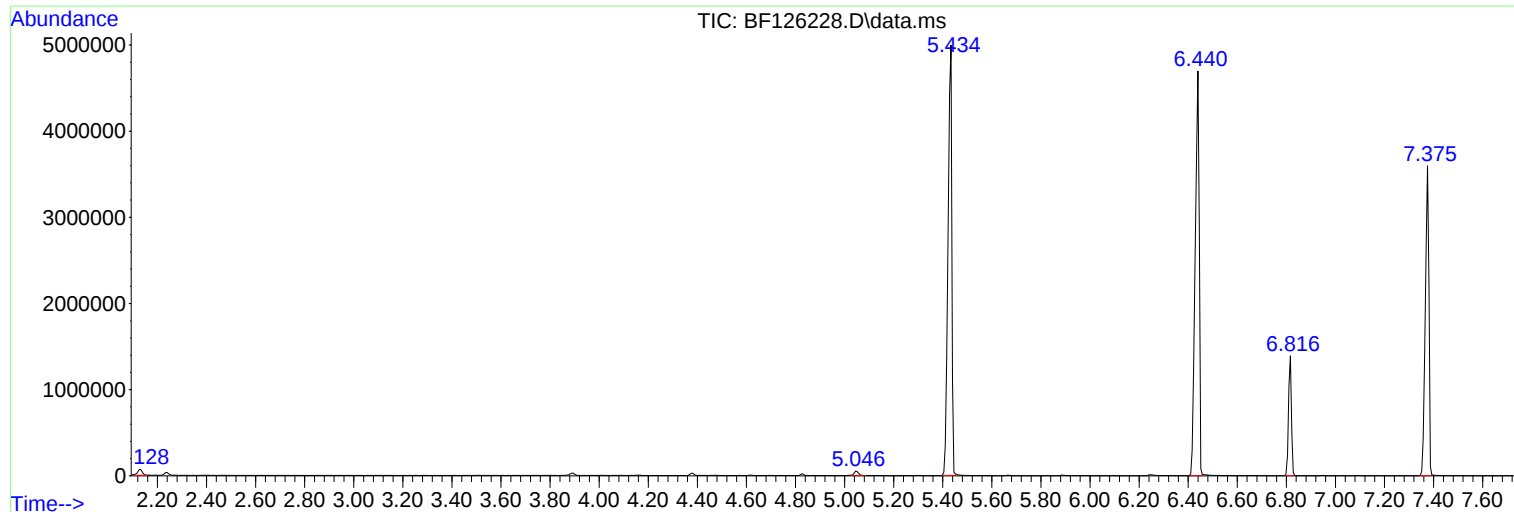
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	12	rVB	69383	88441	1.64%	0.242%
2	5.046	500	503	510	rVB	52216	64594	1.20%	0.177%
3	5.434	563	569	572	rBV	4994513	5398367	99.95%	14.795%
4	6.440	734	740	743	rBV	4696695	5394507	99.88%	14.784%
5	6.816	800	804	807	rBV	1391722	1131349	20.95%	3.101%
6	7.375	893	899	902	rBV	3595790	3678960	68.12%	10.083%
7	8.098	1017	1022	1025	rBV	1638929	1606484	29.74%	4.403%
8	9.175	1200	1205	1208	rBV	5136706	5401084	100.00%	14.802%
9	9.851	1315	1320	1323	rBV	1916420	1639756	30.36%	4.494%
10	10.639	1449	1454	1457	rBV	3092219	2930178	54.25%	8.030%
11	11.333	1568	1572	1575	rBV	1810157	1482808	27.45%	4.064%
12	12.922	1837	1842	1845	rBV	4164252	4150491	76.85%	11.375%
13	13.969	2016	2020	2023	rBV	1072527	946466	17.52%	2.594%
14	14.757	2150	2154	2158	rBV	79340	71809	1.33%	0.197%
15	15.092	2207	2211	2215	rVB	123554	130475	2.42%	0.358%
16	15.410	2260	2265	2270	rBV2	769946	940328	17.41%	2.577%
17	15.468	2270	2275	2280	rVB	167863	226446	4.19%	0.621%
18	15.898	2342	2348	2359	rBV	157783	247338	4.58%	0.678%
19	16.398	2427	2433	2442	rVB	139658	259205	4.80%	0.710%
20	16.704	2477	2485	2499	rVB4	33815	140295	2.60%	0.384%
21	16.980	2526	2532	2544	rBV	107988	220525	4.08%	0.604%
22	17.668	2641	2649	2659	rBV3	80405	215878	4.00%	0.592%
23	18.492	2781	2789	2797	rBV3	44508	122355	2.27%	0.335%

Sum of corrected areas: 36488139

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF126228.D
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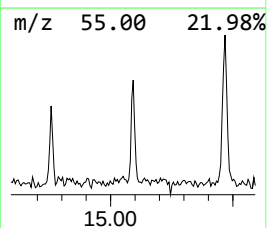
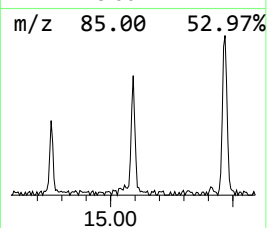
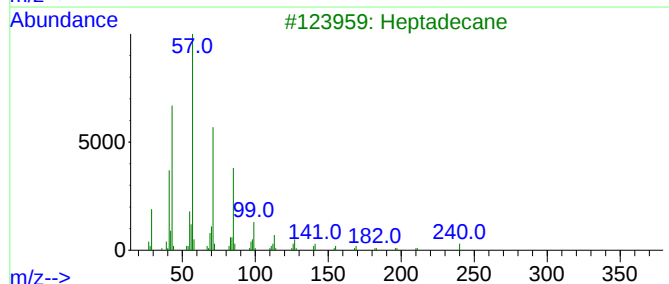
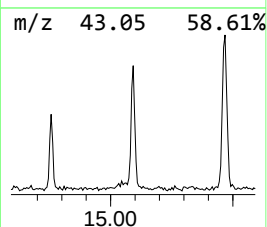
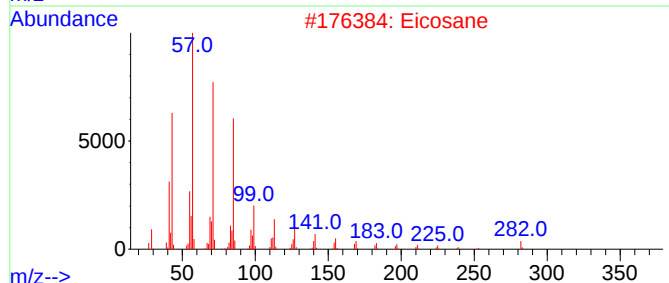
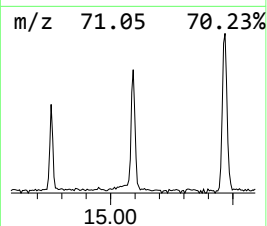
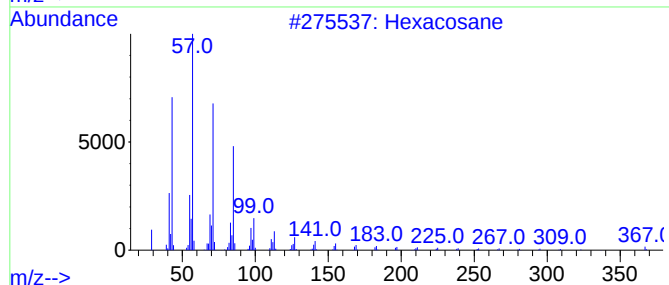
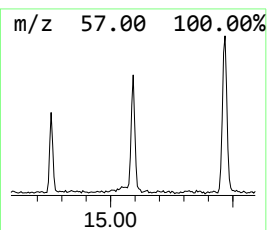
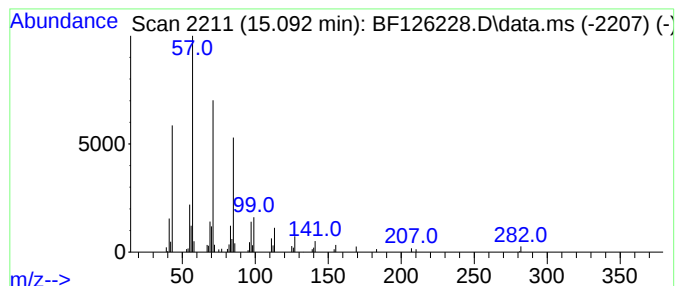
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.78 ng	130475	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Eicosane	282	C20H42	000112-95-8	91
3			Heptadecane	240	C17H36	000629-78-7	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87



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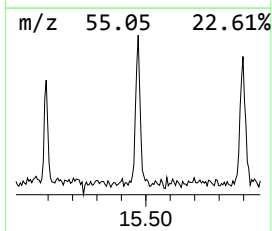
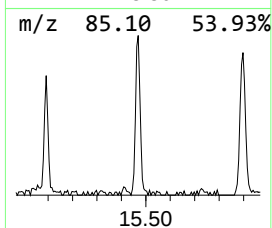
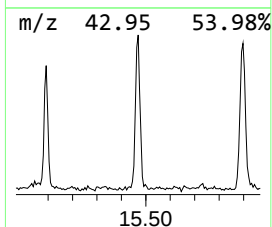
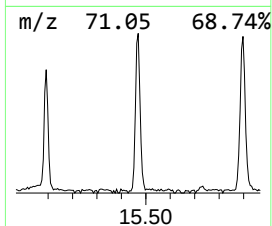
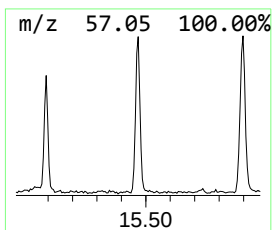
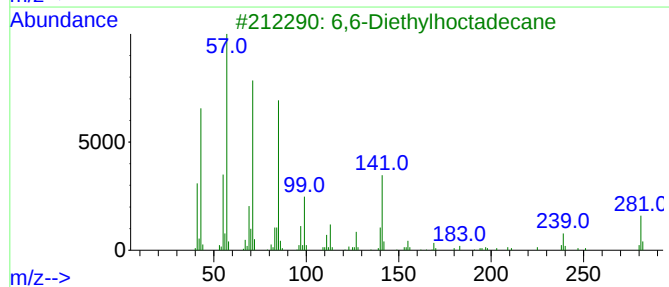
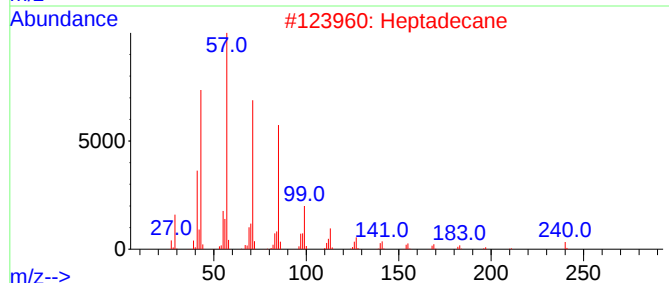
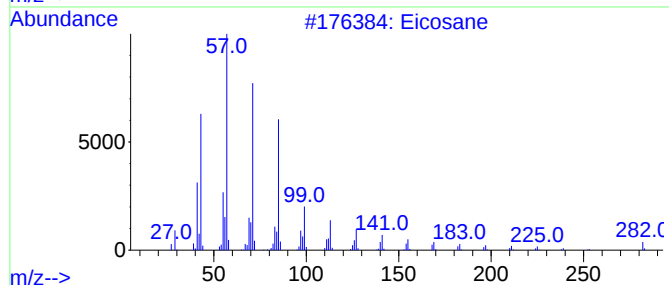
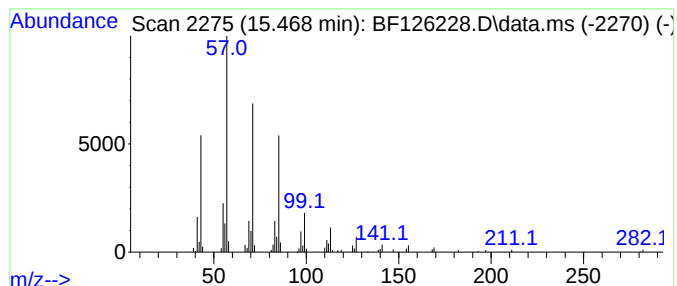
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.469	4.82 ng	226446	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	94
2	Heptadecane			240	C17H36	000629-78-7	91
3	6,6-Diethylhooctadecane			310	C22H46	1000360-41-8	86
4	Sulfurous acid, butyl decyl ester			278	C14H30O3S	1000309-17-7	80
5	Pentacosane			352	C25H52	000629-99-2	80



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Misc :
ALS Vial : 3 Sample Multiplier: 1

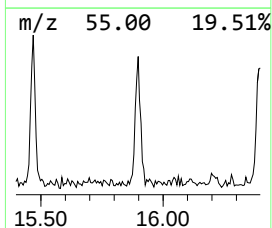
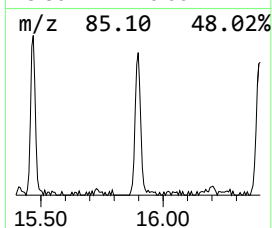
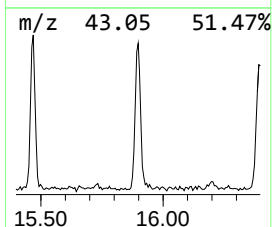
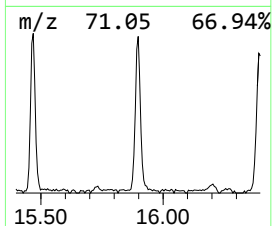
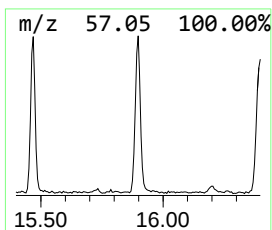
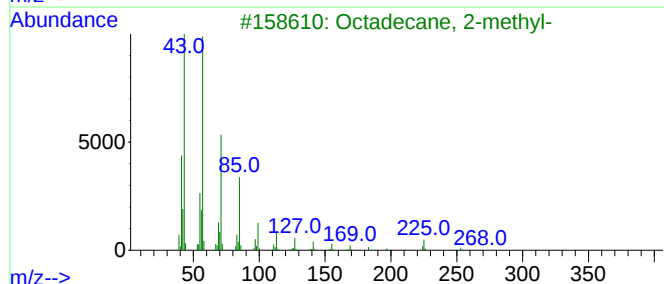
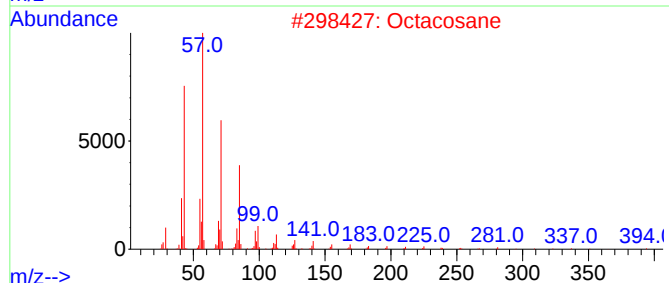
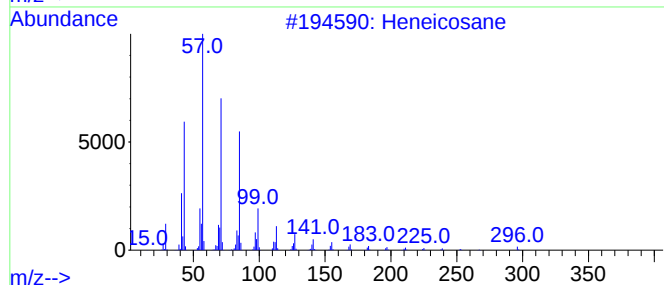
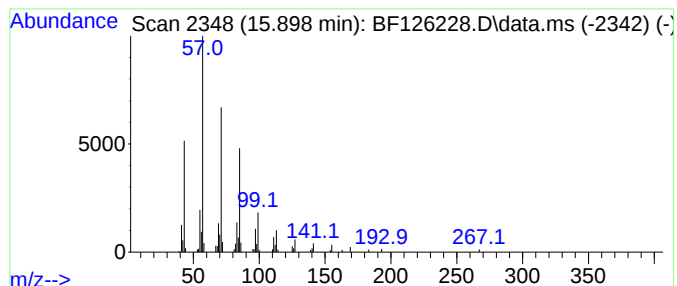
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	5.26 ng	247338	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5			2-Methyltetracosane	352	C25H52	001560-78-7	90



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Misc :
ALS Vial : 3 Sample Multiplier: 1

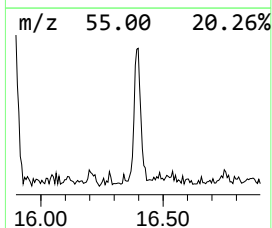
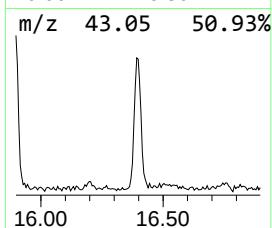
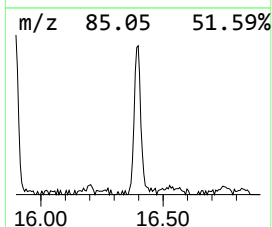
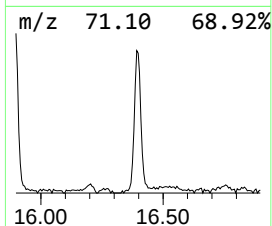
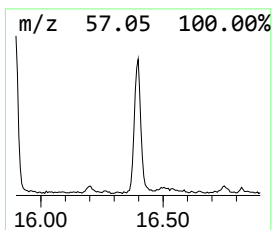
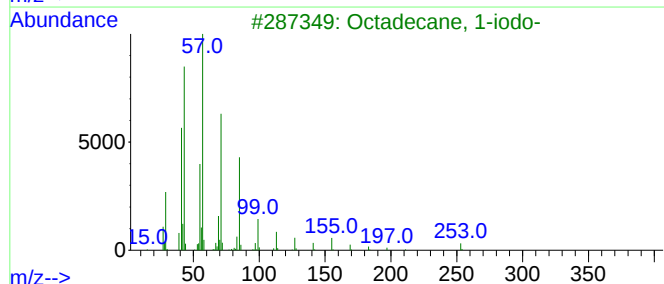
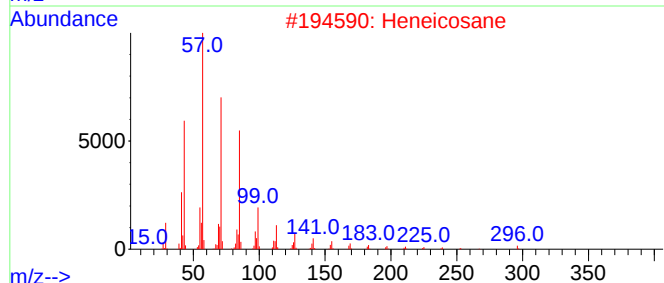
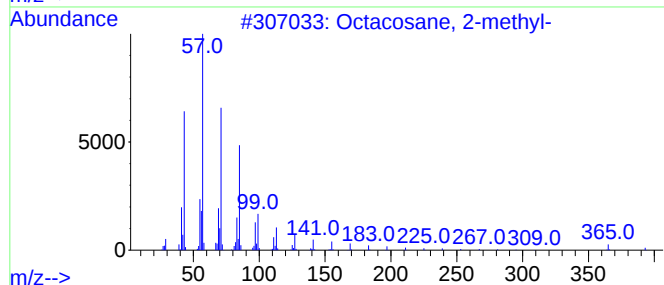
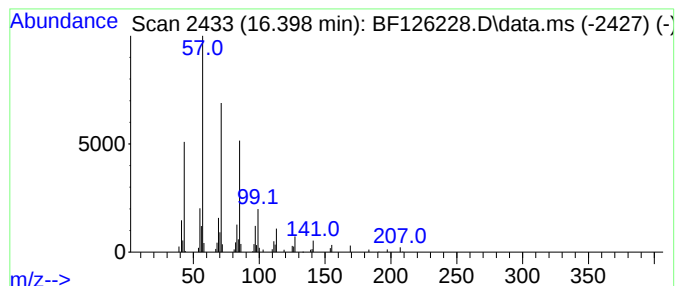
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Peak Number 4 Octacosane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.398	5.51 ng	259205	Perylene-d12	15.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4		Heptadecane	240	C17H36	000629-78-7	87
5		Octacosane	394	C28H58	000630-02-4	83



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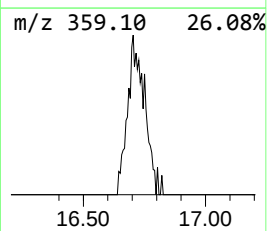
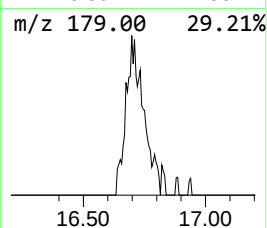
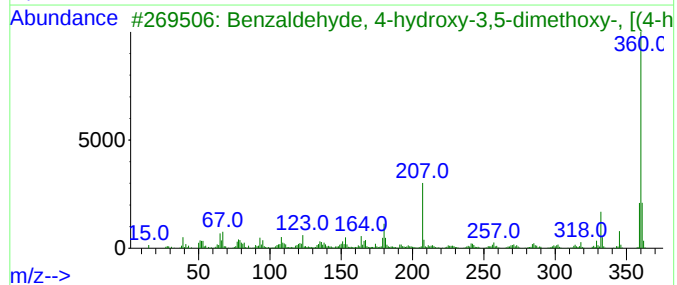
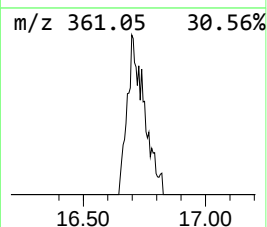
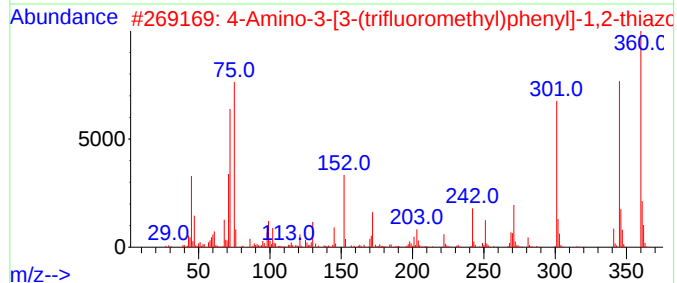
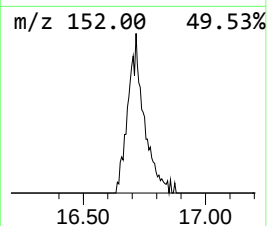
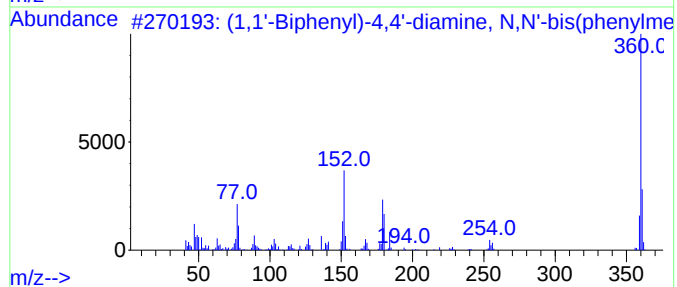
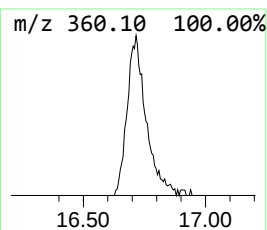
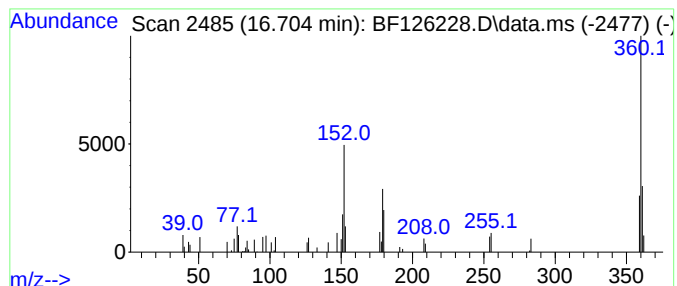
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Peak Number 5 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.704	2.98 ng	140295	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	93
2			4-Amino-3-[3-(trifluoromethyl)ph...	360	C14H15F3N2O2SSi	1010500-98-0	50
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4			Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	43
5			1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43



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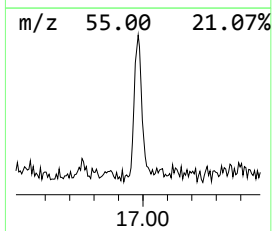
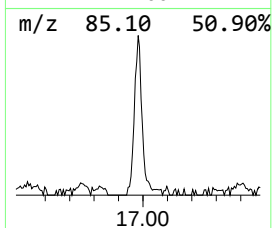
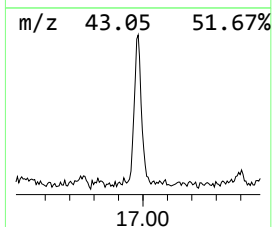
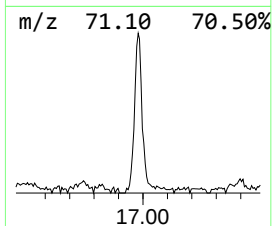
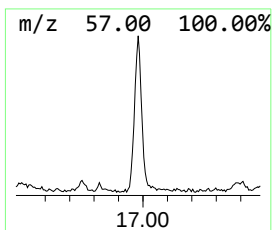
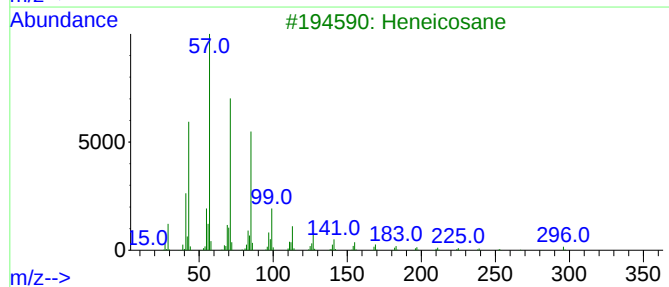
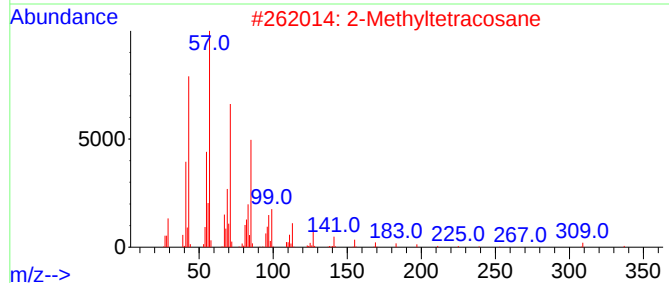
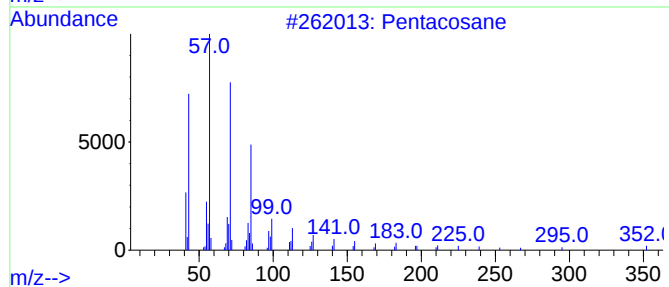
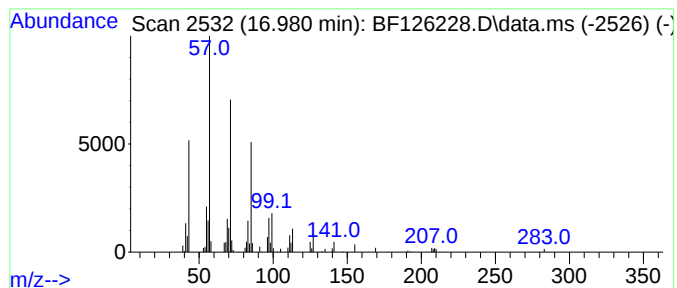
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.980	4.69 ng	220525	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			2-Methyltetracosane	352	C25H52	001560-78-7	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126228.D
Acq On : 17 Dec 2021 11:08
Operator : JU/CG
Sample : PB141306BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

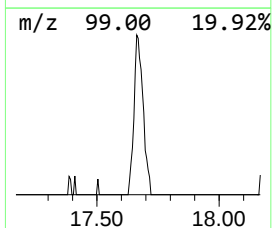
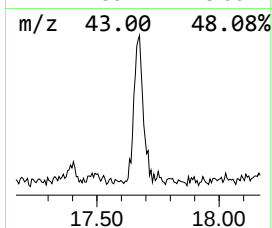
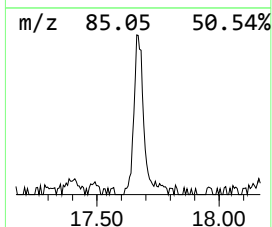
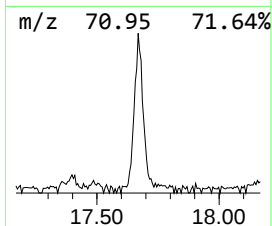
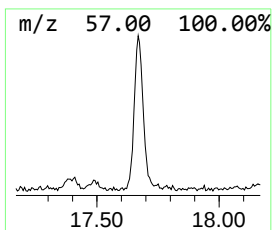
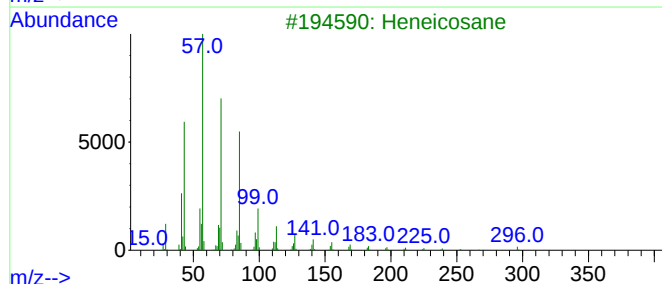
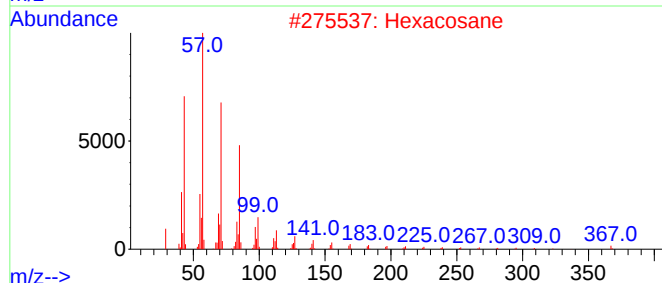
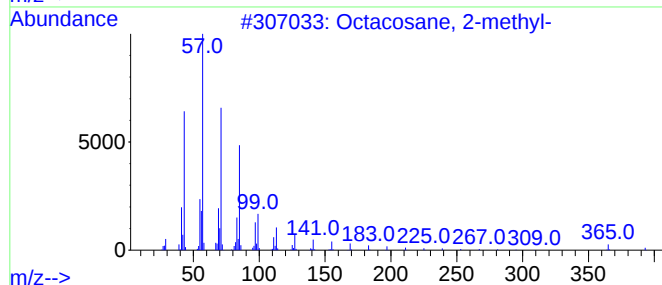
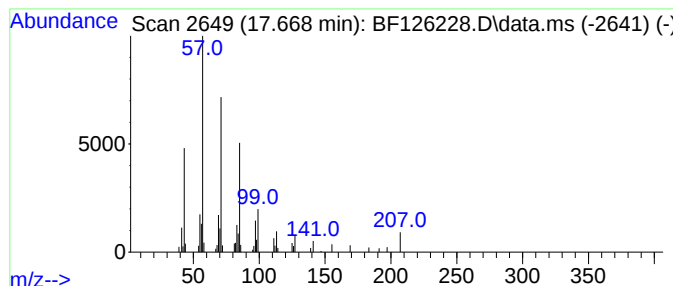
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Bromotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.668	4.59 ng	215878	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-		408	C29H60		001560-98-1	87
2	Hexacosane		366	C26H54		000630-01-3	87
3	Heneicosane		296	C21H44		000629-94-7	87
4	2-Bromotetradecane		276	C14H29Br		074036-95-6	86
5	Octacosane		394	C28H58		000630-02-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126228.D
Acq On : 17 Dec 2021 11:08
Operator : JU/CG
Sample : PB141306BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

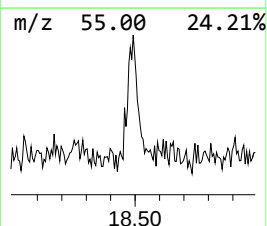
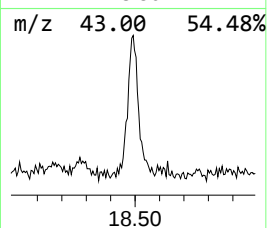
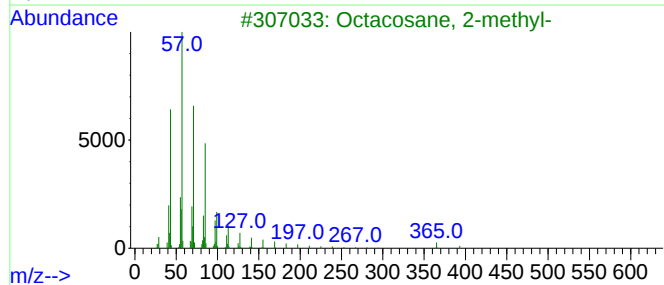
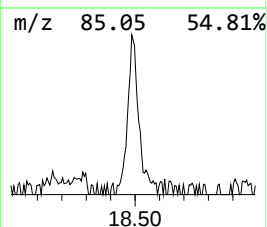
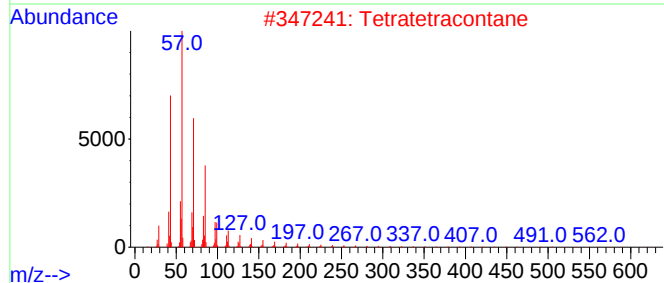
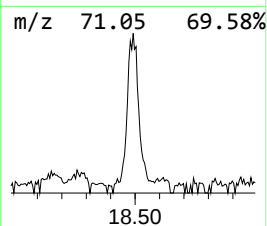
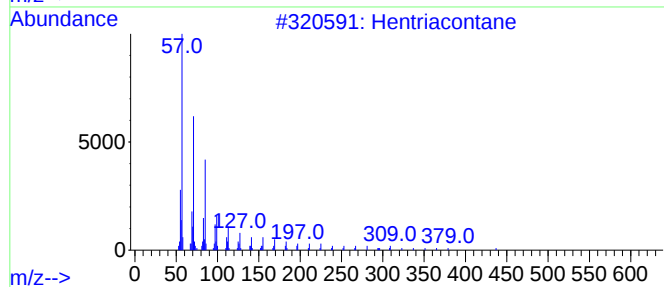
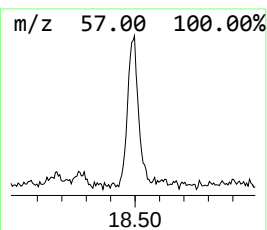
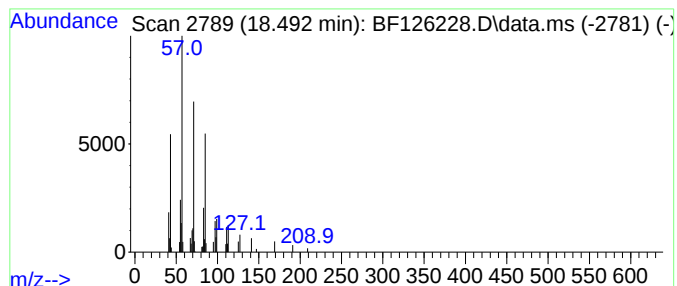
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.492	2.60 ng	122355	Perylene-d12	15.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	90
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121721\
Data File : BF126228.D
Acq On : 17 Dec 2021 11:08
Operator : JU/CG
Sample : PB141306BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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
Hexacosane	15.092	2.8	ng	130475	6	15.410	940328	20.0
Eicosane	15.469	4.8	ng	226446	6	15.410	940328	20.0
Heneicosane	15.898	5.3	ng	247338	6	15.410	940328	20.0
Octacosane, 2-m...	16.398	5.5	ng	259205	6	15.410	940328	20.0
(1,1'-Biphenyl)...	16.704	3.0	ng	140295	6	15.410	940328	20.0
Pentacosane	16.980	4.7	ng	220525	6	15.410	940328	20.0
2-Bromotetradecane	17.668	4.6	ng	215878	6	15.410	940328	20.0
Hentriacontane	18.492	2.6	ng	122355	6	15.410	940328	20.0