

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
 Data File : BF127594.D
 Acq On : 30 Mar 2022 18:11
 Operator : CG\JU
 Sample : N2095-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-01-5.0-6.0

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-BF032122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127594.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	469	472	481	rBV	16809	26600	1.33%	0.177%
2	5.457	536	539	559	rBV	1935227	1965334	98.26%	13.064%
3	6.475	709	712	730	rBV	2033015	1974683	98.73%	13.126%
4	6.833	770	773	781	rBV	599813	523080	26.15%	3.477%
5	7.398	866	869	879	rBV	1369383	1297685	64.88%	8.626%
6	8.116	987	991	1001	rBV	753265	655977	32.80%	4.360%
7	8.686	1086	1088	1093	rBV	28907	25317	1.27%	0.168%
8	9.186	1169	1173	1177	rBV	2399142	2000139	100.00%	13.296%
9	9.251	1182	1184	1188	rVB	59437	52754	2.64%	0.351%
10	9.574	1235	1239	1241	rBV3	20607	23856	1.19%	0.159%
11	9.780	1272	1274	1278	rVB	45147	37536	1.88%	0.250%
12	9.869	1286	1289	1298	rVB	806965	648001	32.40%	4.307%
13	10.280	1353	1359	1362	rBV	54167	58744	2.94%	0.390%
14	10.504	1391	1397	1399	rBV	30578	35435	1.77%	0.236%
15	10.663	1421	1424	1432	rBV	1104866	975612	48.78%	6.485%
16	10.757	1437	1440	1449	rVB	69960	90810	4.54%	0.604%
17	11.204	1513	1516	1518	rBV	64797	47274	2.36%	0.314%
18	11.233	1518	1521	1530	rVB4	37413	50019	2.50%	0.332%
19	11.363	1540	1543	1546	rBV	641173	548017	27.40%	3.643%
20	11.392	1546	1548	1551	rVB2	39963	41120	2.06%	0.273%
21	11.633	1586	1589	1591	rBV	62015	47477	2.37%	0.316%
22	11.733	1603	1606	1610	rVB	70231	63350	3.17%	0.421%
23	11.874	1627	1630	1638	rBV6	44762	84111	4.21%	0.559%
24	12.039	1655	1658	1661	rBV	70882	56751	2.84%	0.377%
25	12.427	1719	1724	1730	rBV2	69665	103319	5.17%	0.687%
26	12.798	1785	1787	1789	rBV	55231	44637	2.23%	0.297%
27	12.915	1804	1807	1808	rBV2	25832	28596	1.43%	0.190%
28	12.945	1808	1812	1815	rVV	1939311	1618805	80.93%	10.761%
29	13.157	1845	1848	1851	rBV	57574	50208	2.51%	0.334%
30	13.280	1866	1869	1873	rBV5	20394	25937	1.30%	0.172%
31	13.498	1903	1906	1912	rBV2	62035	74423	3.72%	0.495%
32	13.833	1960	1963	1975	rVB5	95531	225406	11.27%	1.498%
33	14.015	1990	1994	2003	rBV	517491	523976	26.20%	3.483%
34	14.145	2014	2016	2019	rVB	41840	32003	1.60%	0.213%
35	14.451	2065	2068	2072	rBV	68613	74843	3.74%	0.498%
36	14.756	2117	2120	2124	rVB	55299	59712	2.99%	0.397%

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SB-01-5.0-6.0

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-BF032122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.827	2129	2132	2136	rVB	158742	157168	7.86%	1.045%
38	15.086	2173	2176	2180	rVB	74523	81280	4.06%	0.540%
39	15.462	2237	2240	2243	rBV	72249	87216	4.36%	0.580%
40	15.498	2243	2246	2256	rVB	289178	380287	19.01%	2.528%
41	16.151	2354	2357	2367	rVB5	77256	146201	7.31%	0.972%

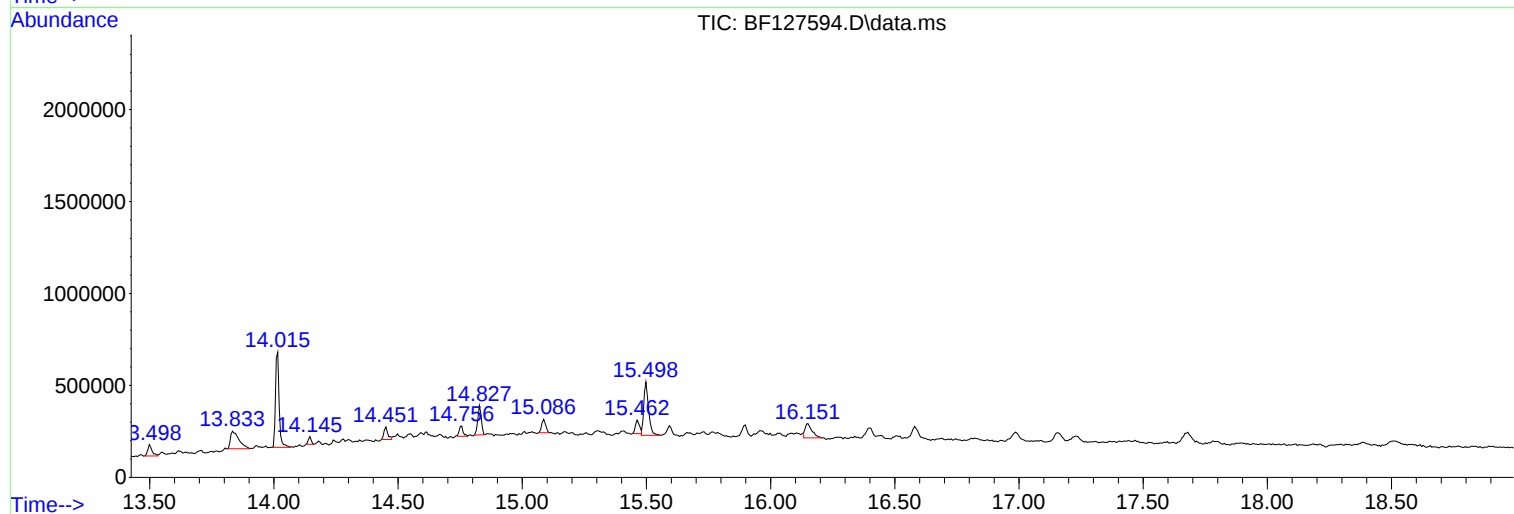
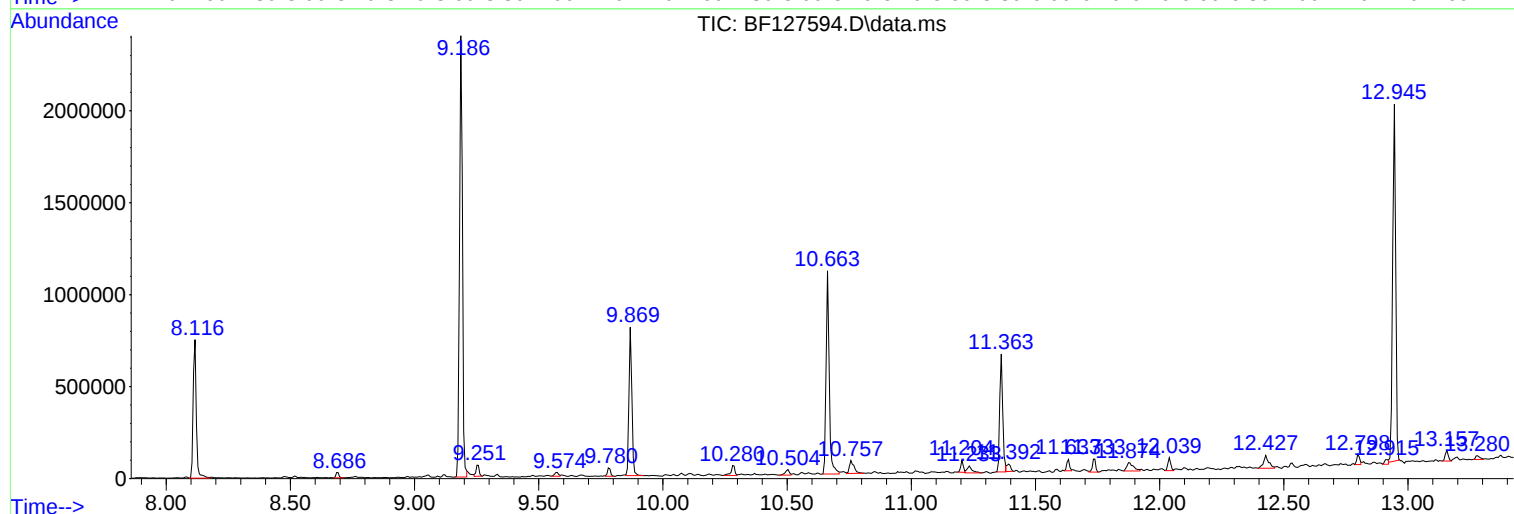
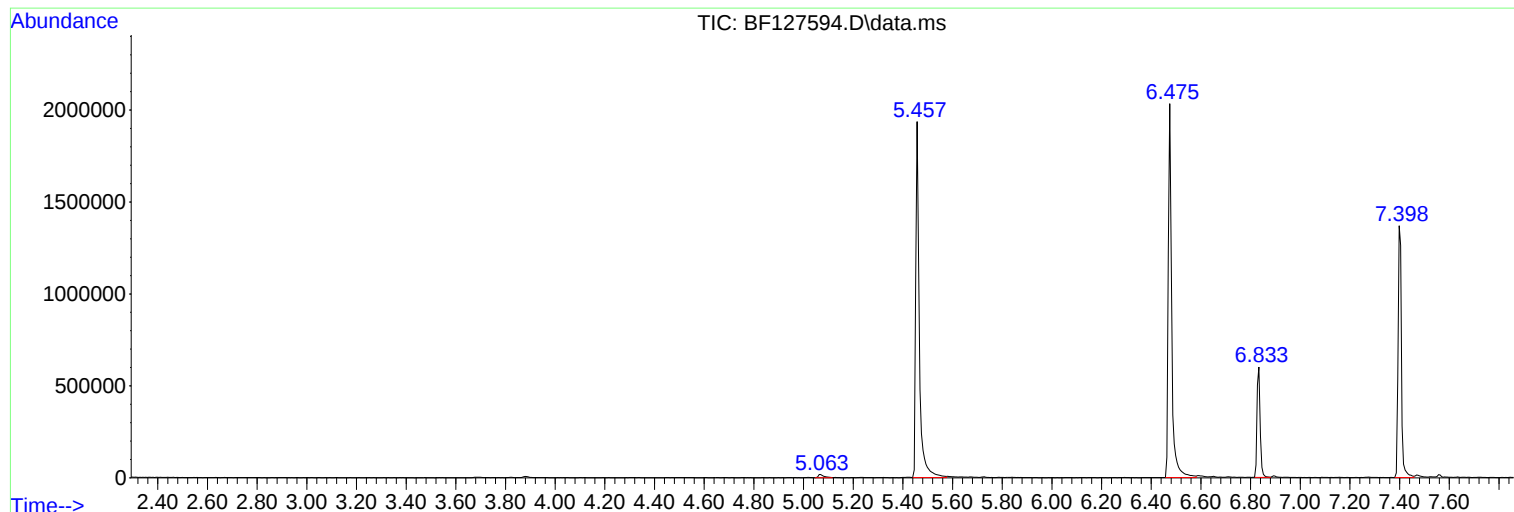
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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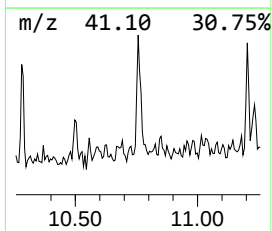
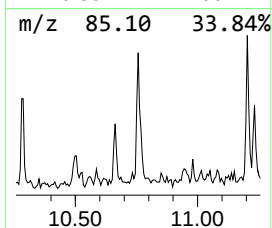
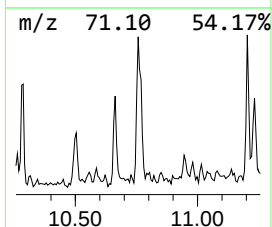
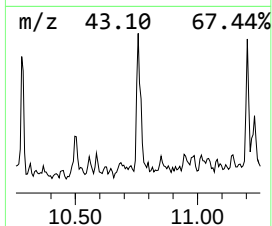
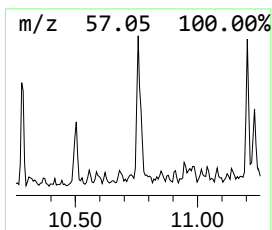
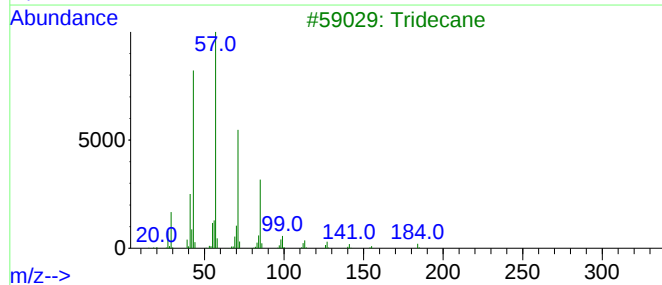
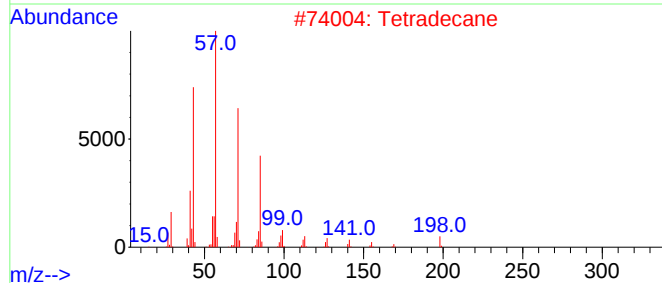
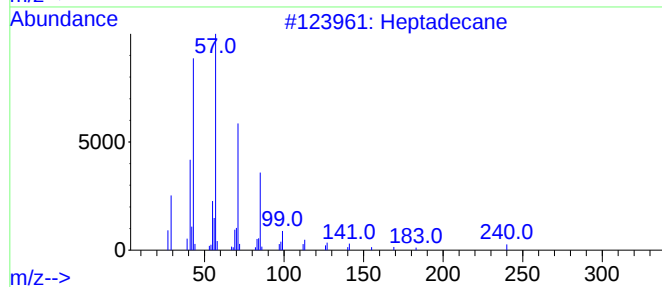
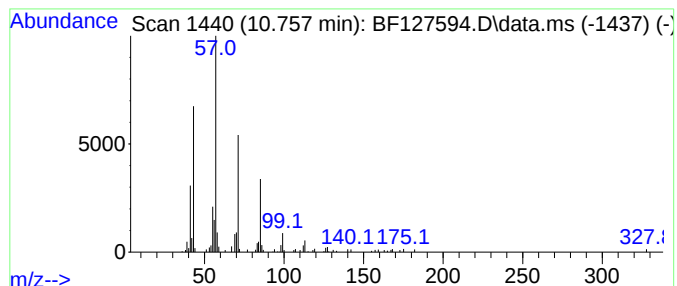
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	3.31 ng	90810	Phenanthrene-d10	11.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	86
2		Tetradecane	198	C14H30	000629-59-4	86
3		Tridecane	184	C13H28	000629-50-5	86
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	78
5		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	64



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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-5.0-6.0

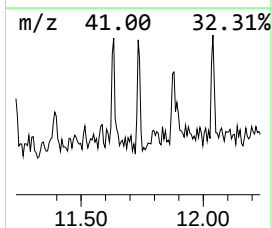
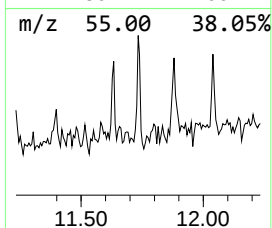
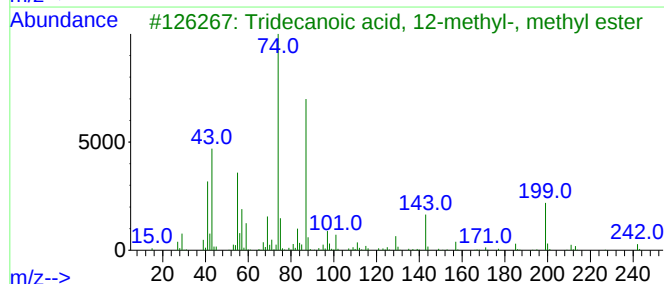
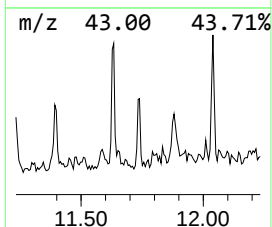
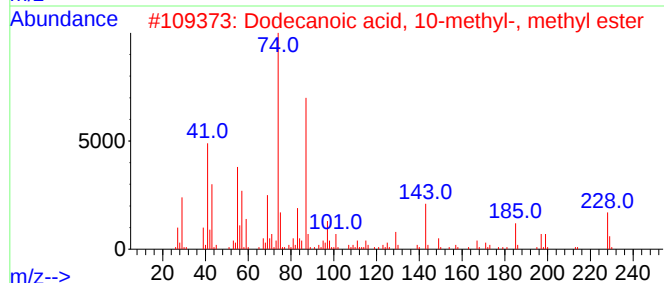
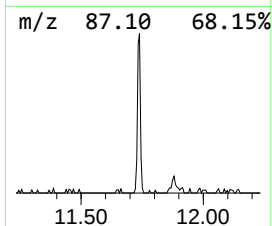
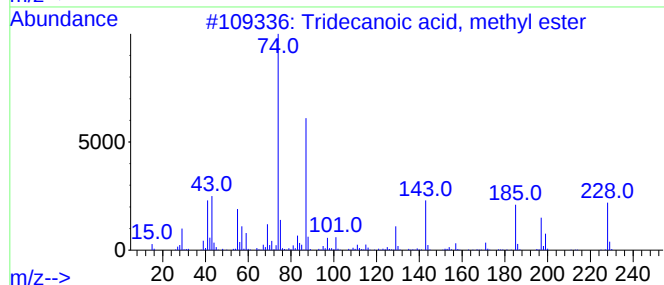
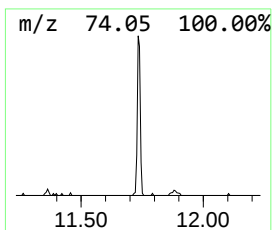
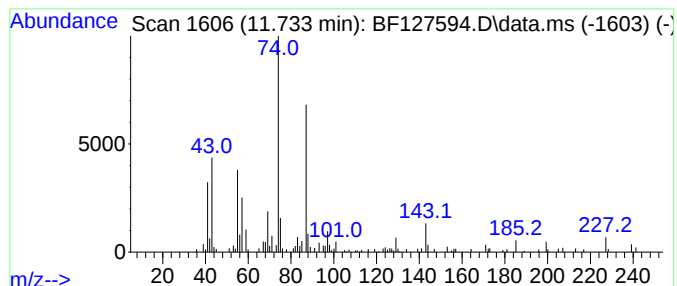
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Tridecanoic acid, methyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.733	2.31 ng	63350	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
2			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	90
3			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	78
4			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72
5			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	72



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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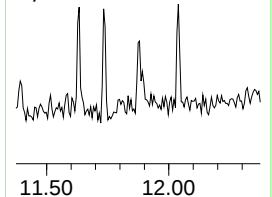
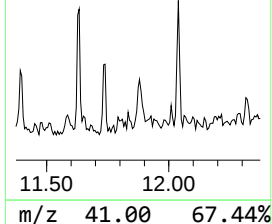
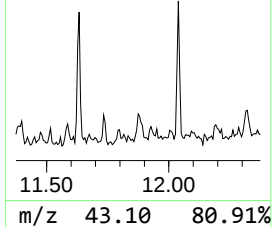
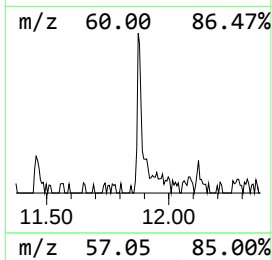
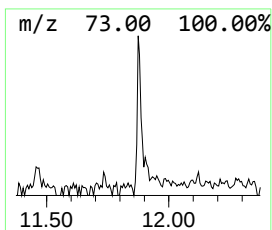
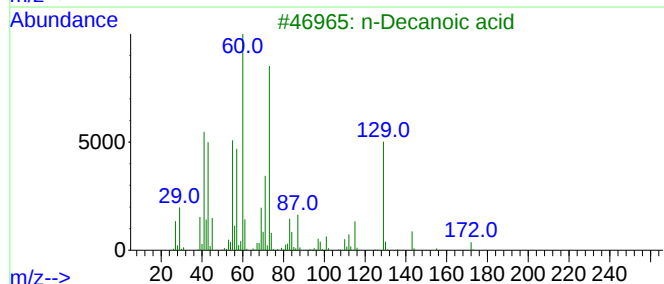
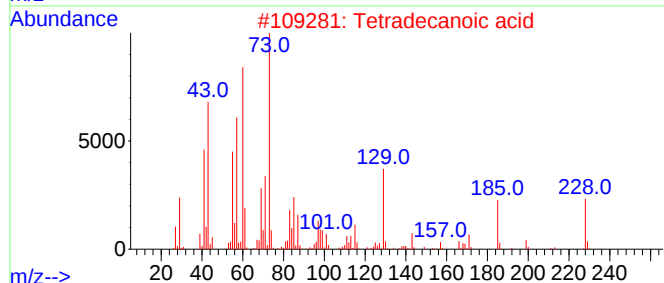
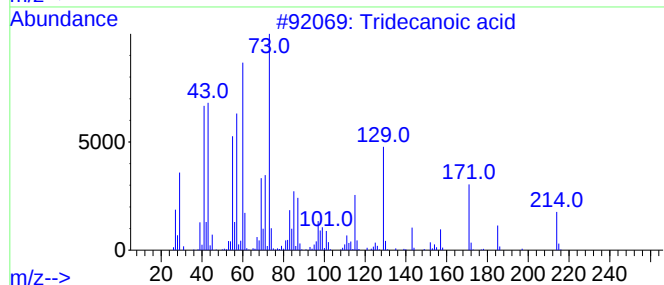
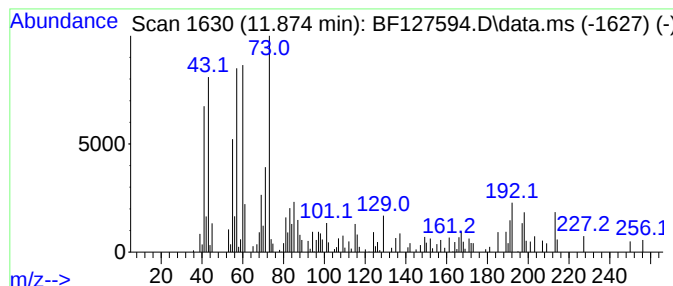
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.874	3.07 ng	84111	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	83
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	58
4			Undecanoic acid	186	C11H22O2	000112-37-8	52
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50



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Instrument :
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ClientSampleId :
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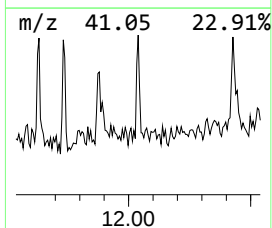
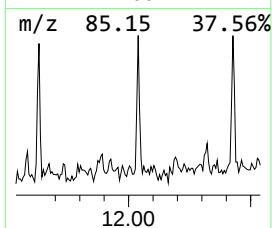
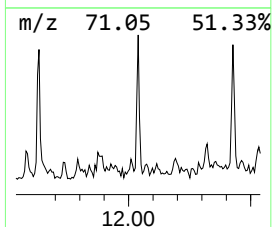
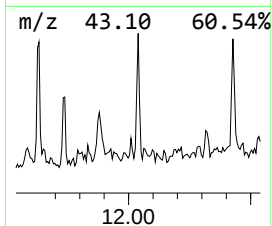
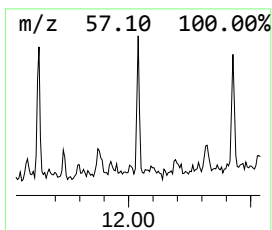
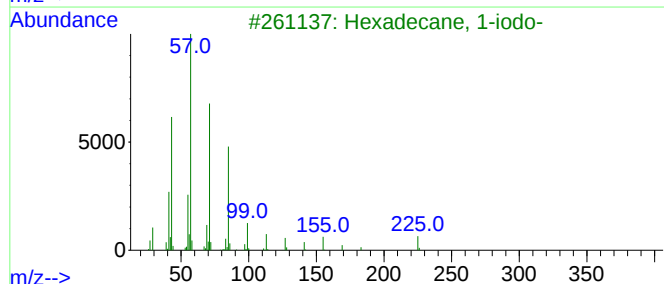
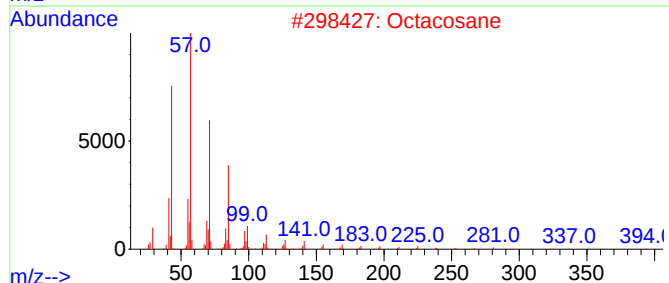
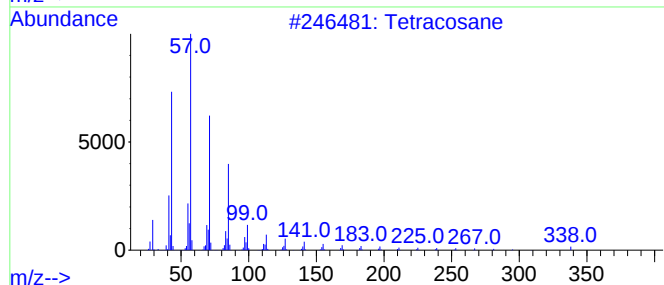
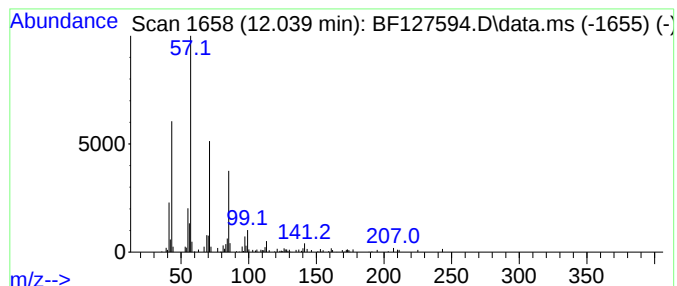
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	2.07 ng	56751	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	87
2			Octacosane	394	C28H58	000630-02-4	87
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
4			Pentadecane	212	C15H32	000629-62-9	80
5			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80



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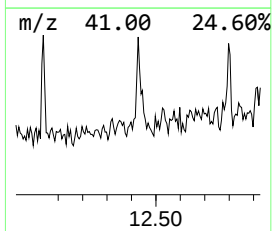
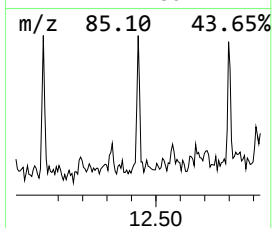
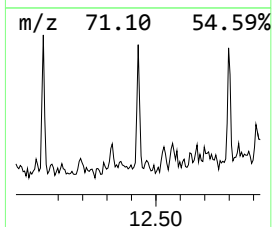
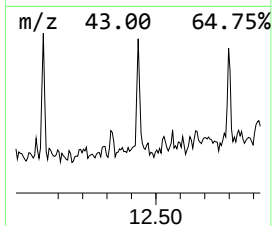
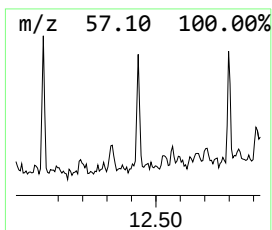
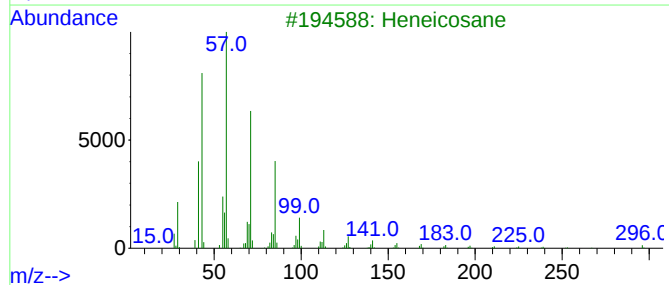
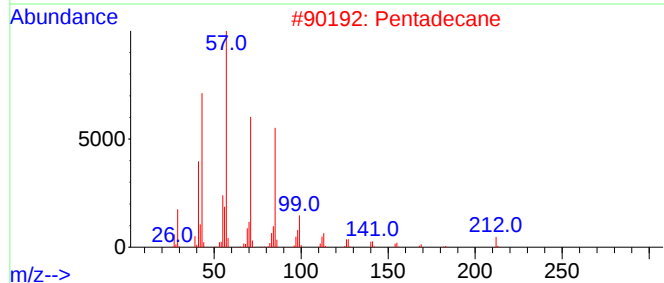
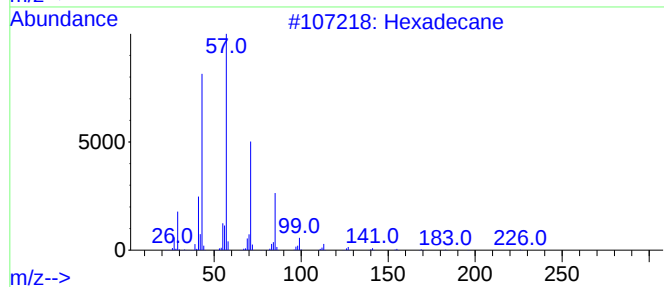
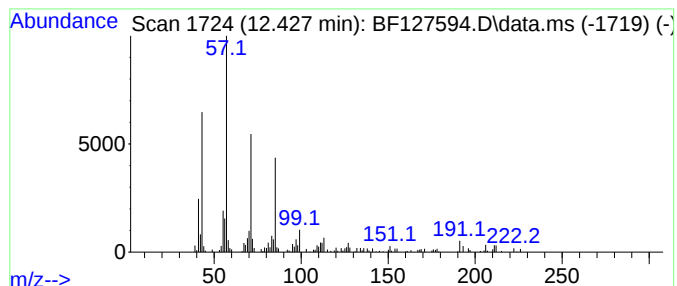
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	3.77 ng	103319	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	94
2			Pentadecane	212	C15H32	000629-62-9	93
3			Heneicosane	296	C21H44	000629-94-7	80
4			Tridecane	184	C13H28	000629-50-5	80
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
Data File : BF127594.D
Acq On : 30 Mar 2022 18:11
Operator : CG\JU
Sample : N2095-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-5.0-6.0

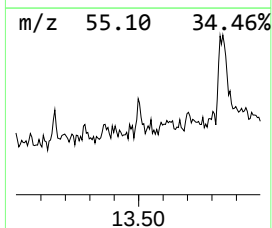
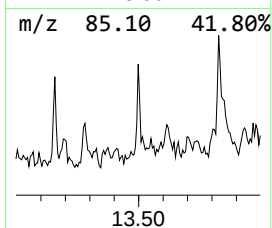
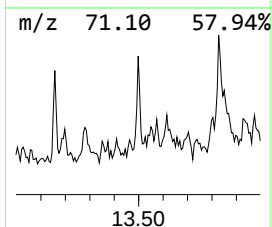
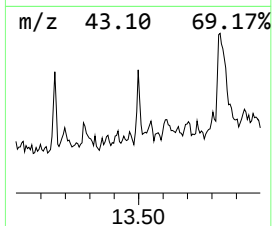
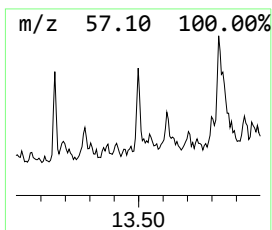
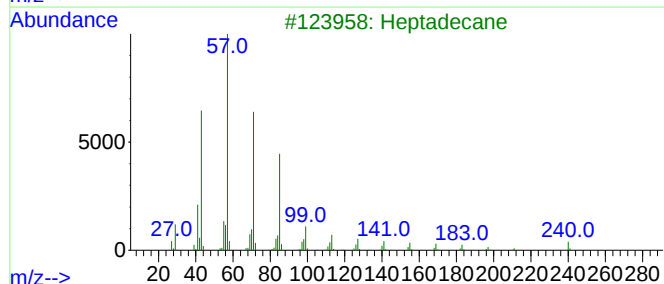
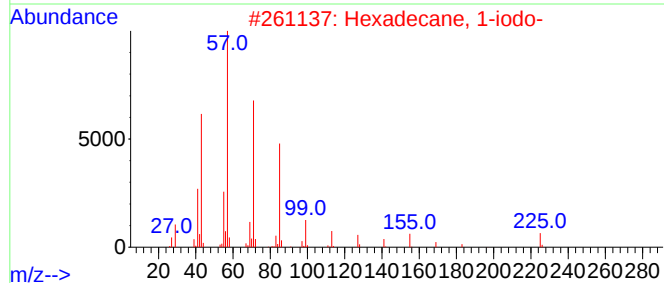
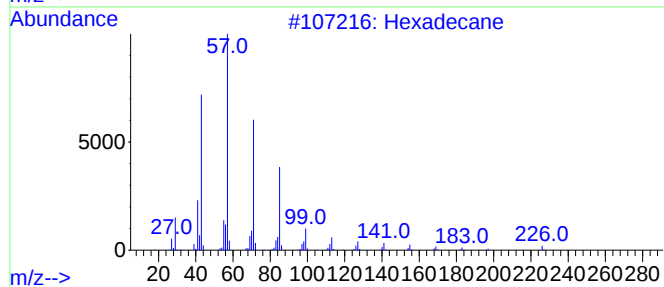
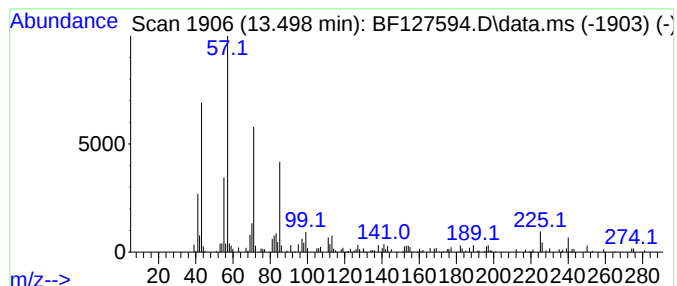
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.498	2.84 ng	74423	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	83
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
3			Heptadecane	240	C17H36	000629-78-7	80
4			Tetradecane	198	C14H30	000629-59-4	76
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
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Sample : N2095-01
Misc :
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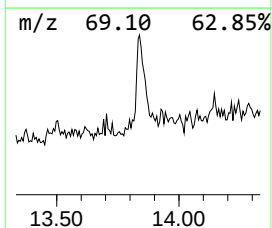
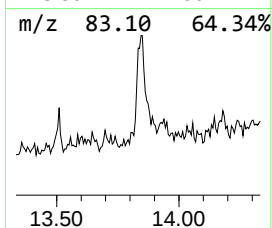
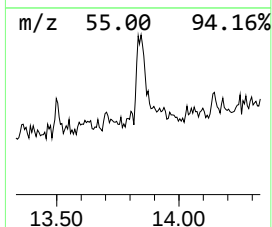
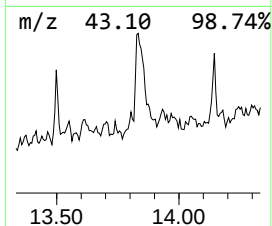
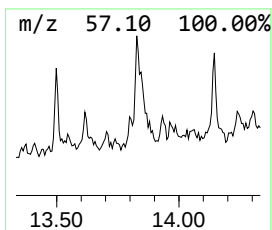
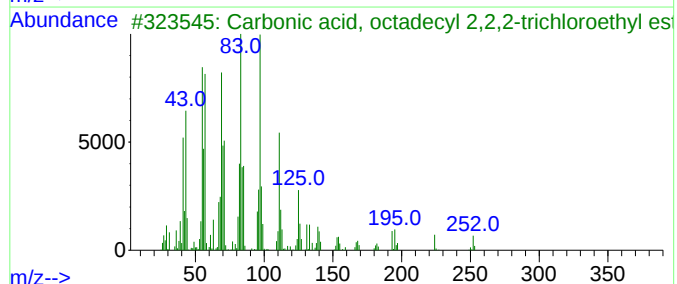
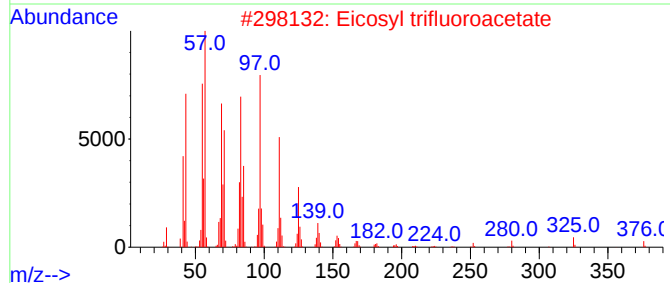
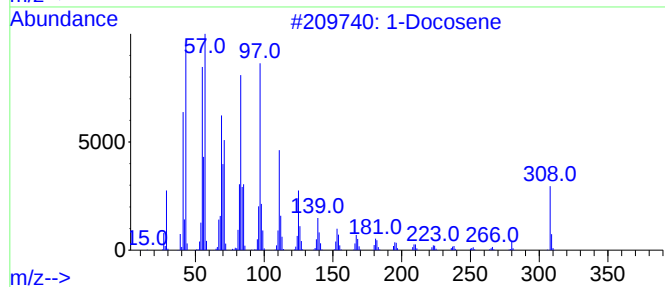
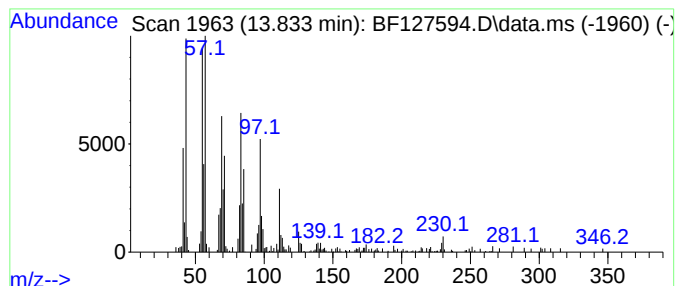
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.833	8.60 ng	225406	Chrysene-d12	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	93
2	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	90
4	Z-5-Nonadecene	266	C19H38	1000131-11-8	89
5	1-Nonadecene	266	C19H38	018435-45-5	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
Data File : BF127594.D
Acq On : 30 Mar 2022 18:11
Operator : CG\JU
Sample : N2095-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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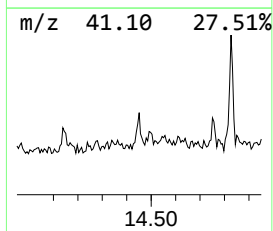
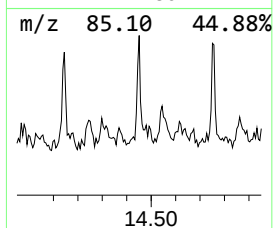
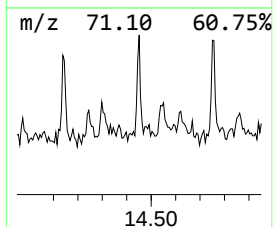
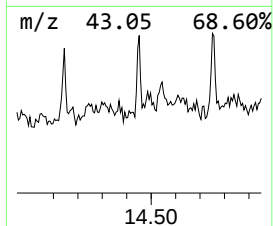
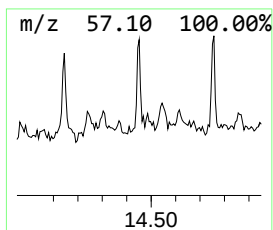
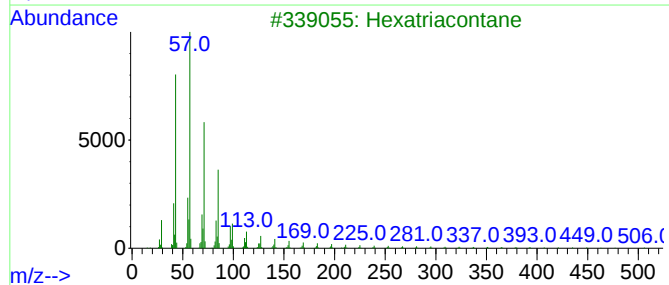
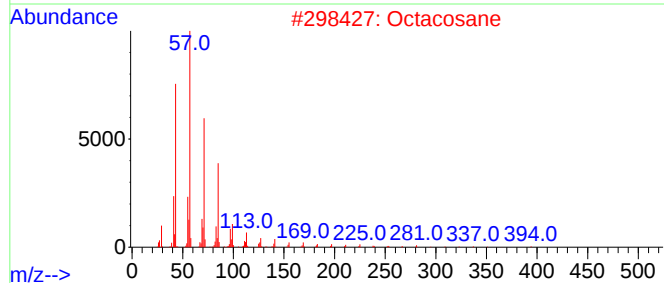
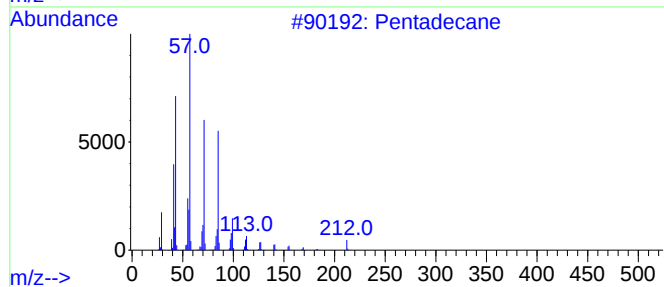
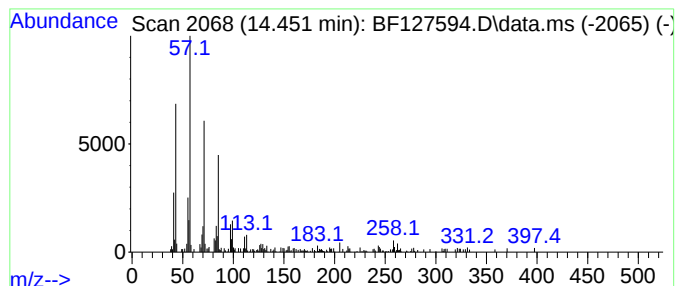
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	2.86 ng	74843	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	90
2			Octacosane	394	C28H58	000630-02-4	83
3			Hexatriacontane	507	C36H74	000630-06-8	83
4			Tridecane	184	C13H28	000629-50-5	81
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
Data File : BF127594.D
Acq On : 30 Mar 2022 18:11
Operator : CG\JU
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ALS Vial : 17 Sample Multiplier: 1

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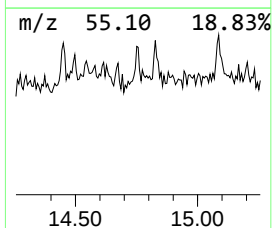
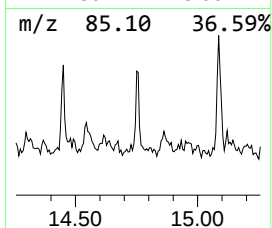
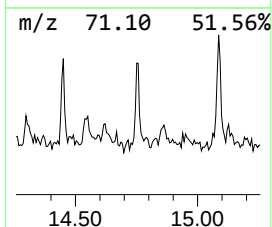
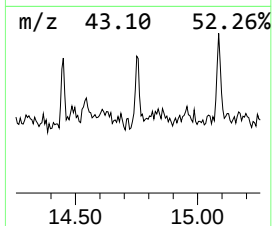
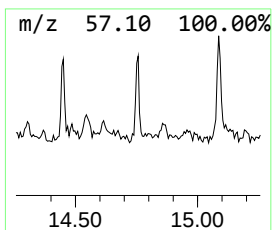
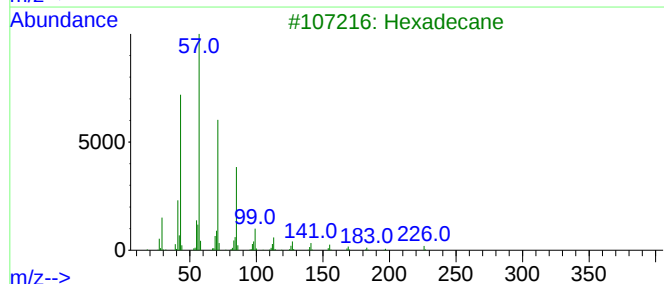
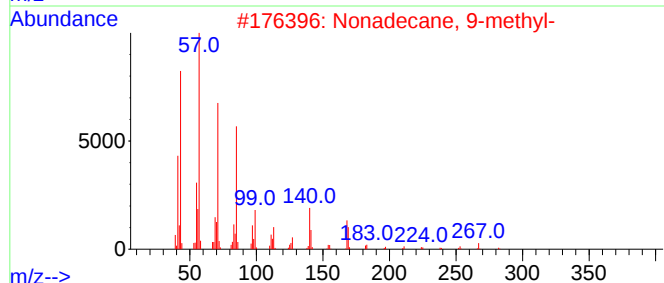
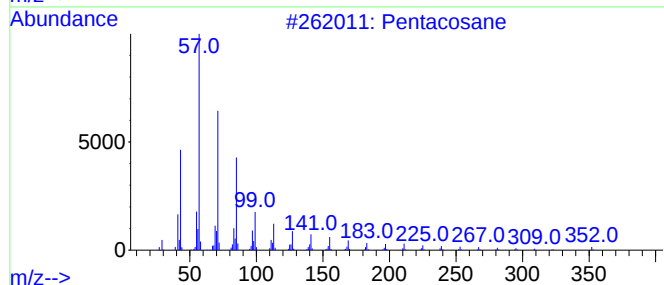
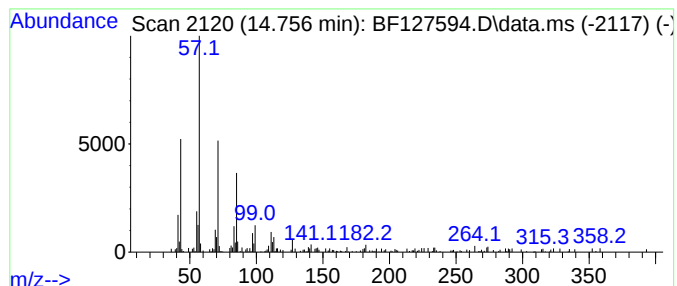
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.757	2.28 ng	59712	Chrysene-d12	14.015

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	91
2		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	89
3		Hexadecane	226	C16H34	000544-76-3	81
4		Octacosane	394	C28H58	000630-02-4	81
5		1-Iodoundecane	282	C11H23I	004282-44-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
Data File : BF127594.D
Acq On : 30 Mar 2022 18:11
Operator : CG\JU
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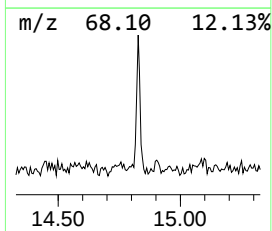
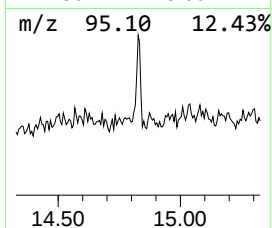
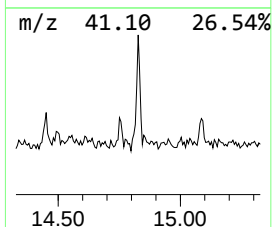
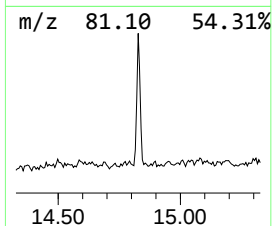
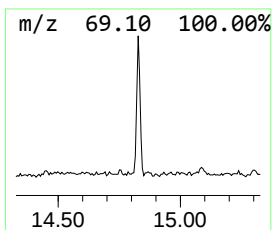
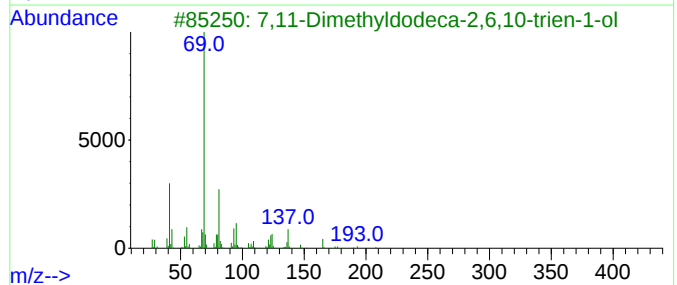
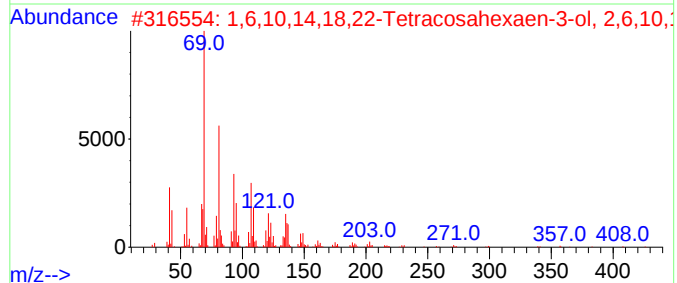
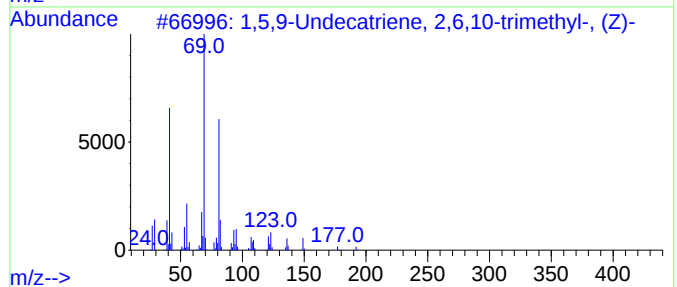
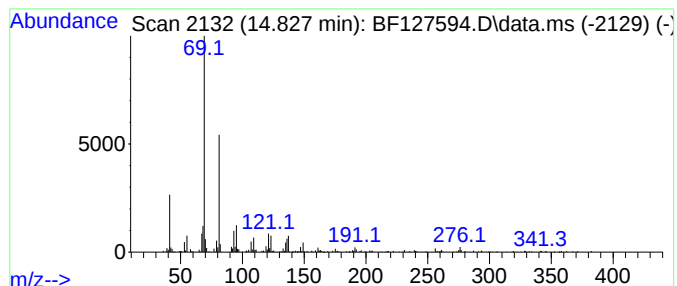
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.827	8.27 ng	157168	Perylene-d12	15.498	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
2	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H500	097232-74-1	78
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H240	125529-10-4	64
4	trans-Farnesol	222	C15H260	000106-28-5	64
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
Data File : BF127594.D
Acq On : 30 Mar 2022 18:11
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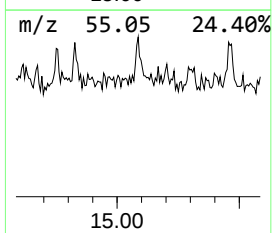
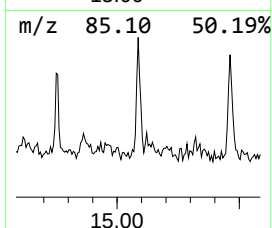
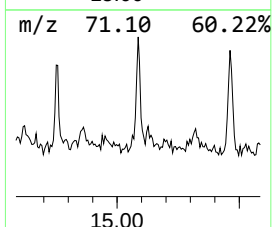
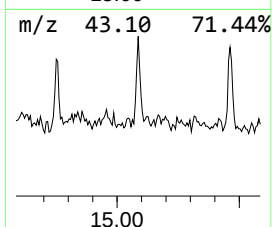
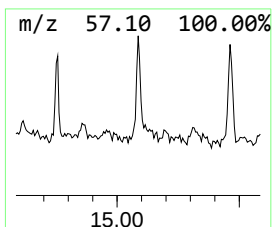
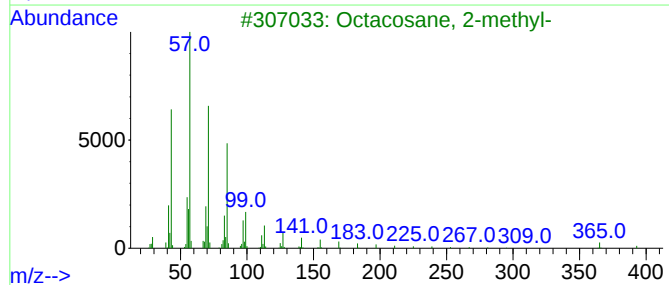
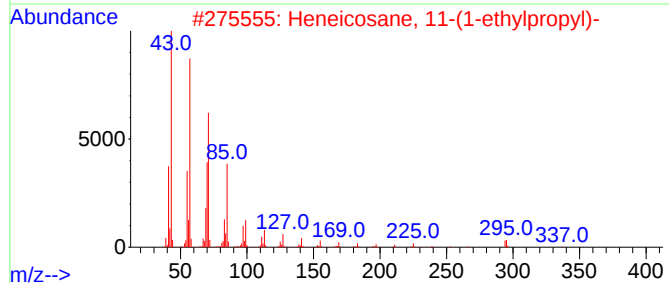
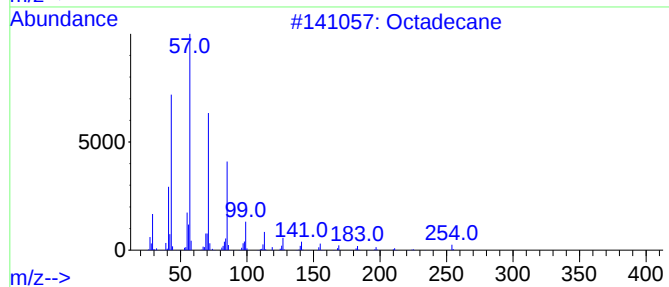
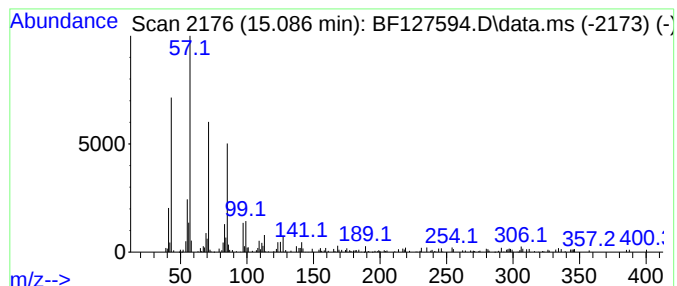
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	4.27 ng	81280	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	90
2			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
4			Tetracosane	338	C24H50	000646-31-1	86
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
Data File : BF127594.D
Acq On : 30 Mar 2022 18:11
Operator : CG\JU
Sample : N2095-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-01-5.0-6.0

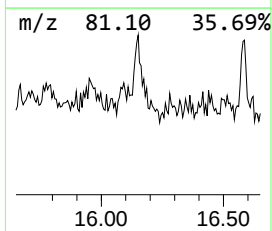
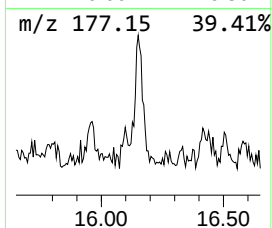
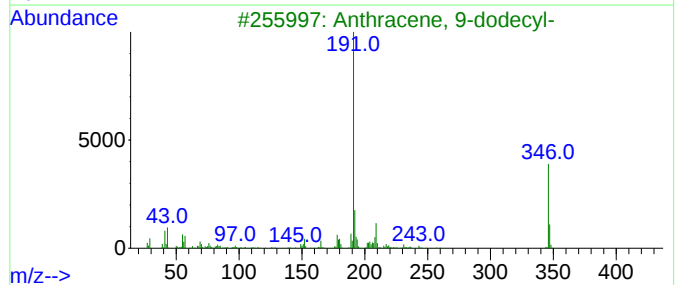
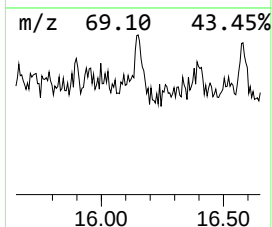
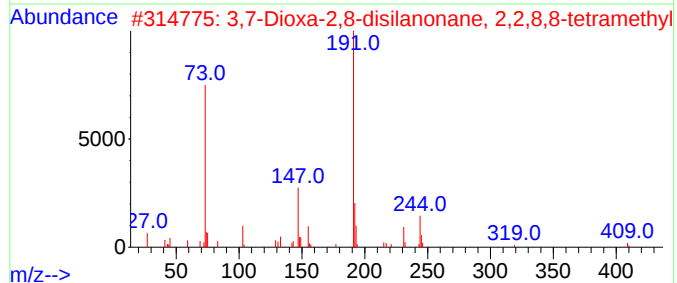
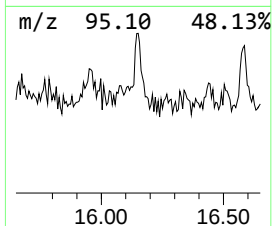
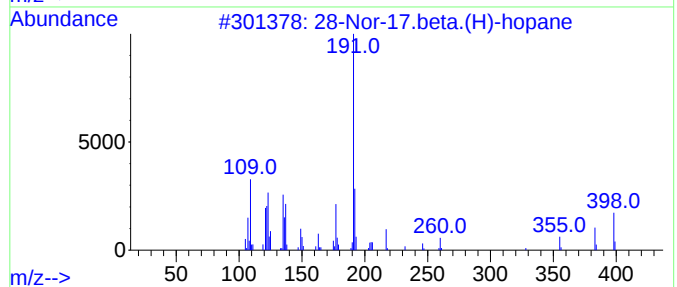
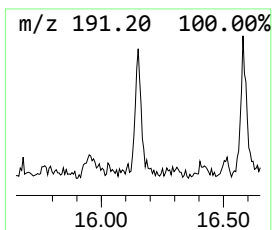
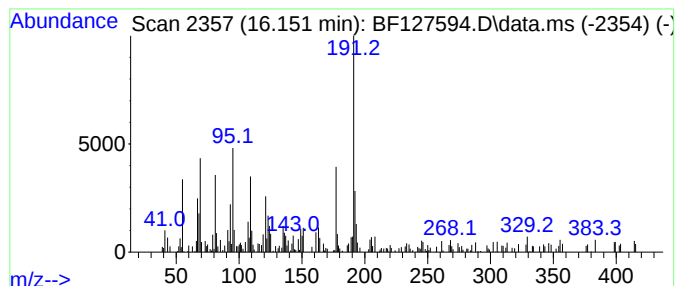
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 28-Nor-17.beta.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.151	7.69 ng	146201	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	52
2			3,7-Dioxa-2,8-disilanonane, 2,2,...	424	C17H44O4Si4	002114-25-2	35
3			Anthracene, 9-dodecyl-	346	C26H34	002883-70-7	30
4			Benzamide, 2-fluoro-6-trifluorom...	317	C16H19F4NO	1000446-40-0	30
5			Propenamide, 3-(3-methoxyphenyl)...	191	C11H13NO2	1000259-85-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF033022\
Data File : BF127594.D
Acq On : 30 Mar 2022 18:11
Operator : CG\JU
Sample : N2095-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-01-5.0-6.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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
Heptadecane	10.757	3.3	ng	90810	4	11.363	548017	20.0
Tridecanoic aci...	11.733	2.3	ng	63350	4	11.363	548017	20.0
Tridecanoic acid	11.874	3.1	ng	84111	4	11.363	548017	20.0
Tetracosane	12.039	2.1	ng	56751	4	11.363	548017	20.0
Hexadecane	12.427	3.8	ng	103319	4	11.363	548017	20.0
Hexadecane, 1-i...	13.498	2.8	ng	74423	5	14.015	523976	20.0
1-Docosene	13.833	8.6	ng	225406	5	14.015	523976	20.0
Pentadecane	14.451	2.9	ng	74843	5	14.015	523976	20.0
Pentacosane	14.757	2.3	ng	59712	5	14.015	523976	20.0
1,5,9-Undecatri...	14.827	8.3	ng	157168	6	15.498	380287	20.0
Octadecane	15.086	4.3	ng	81280	6	15.498	380287	20.0
28-Nor-17.beta....	16.151	7.7	ng	146201	6	15.498	380287	20.0