

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
 Data File : BF130028.D
 Acq On : 26 Aug 2022 20:19
 Operator : CG\JU
 Sample : N4379-08
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04-12-13

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-BF081422.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130028.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	454	458	473	rBV	79994	124848	4.11%	0.615%
2	5.393	524	528	549	rBV	2681673	2876704	94.75%	14.171%
3	6.410	698	701	716	rBV	2651508	2819325	92.86%	13.888%
4	6.745	755	758	767	rBV	896221	731856	24.11%	3.605%
5	7.322	852	856	865	rBV	1854761	1795966	59.16%	8.847%
6	8.028	973	976	981	rBV	1122141	895462	29.50%	4.411%
7	9.104	1155	1159	1162	rBV	3820800	3035958	100.00%	14.955%
8	9.781	1271	1274	1278	rBV	1067093	815719	26.87%	4.018%
9	10.575	1406	1409	1423	rBV	1525767	1377244	45.36%	6.784%
10	11.269	1524	1527	1531	rBV	798918	674213	22.21%	3.321%
11	11.651	1588	1592	1595	rBV	65315	60980	2.01%	0.300%
12	11.792	1613	1616	1620	rBV2	44009	53029	1.75%	0.261%
13	12.357	1703	1712	1714	rBV	167787	211537	6.97%	1.042%
14	12.439	1724	1726	1731	rVB	72594	57794	1.90%	0.285%
15	12.498	1732	1736	1739	rBV2	95586	90550	2.98%	0.446%
16	12.657	1759	1763	1769	rBV	467017	381145	12.55%	1.878%
17	12.851	1792	1796	1802	rBV	2727444	2604042	85.77%	12.827%
18	13.286	1866	1870	1873	rVB	47021	51770	1.71%	0.255%
19	13.798	1952	1957	1961	rBV5	43119	95719	3.15%	0.472%
20	13.916	1974	1977	1982	rBV	739401	665319	21.91%	3.277%
21	14.004	1988	1992	1996	rBV	70459	77488	2.55%	0.382%
22	14.357	2049	2052	2056	rBV	46915	42585	1.40%	0.210%
23	14.651	2100	2102	2106	rBV	42708	45413	1.50%	0.224%
24	14.727	2112	2115	2118	rBV	47377	49326	1.62%	0.243%
25	14.974	2154	2157	2161	rVB	47935	48678	1.60%	0.240%
26	15.327	2215	2217	2220	rBV	32954	39593	1.30%	0.195%
27	15.363	2220	2223	2228	rVB2	421711	478637	15.77%	2.358%
28	15.739	2284	2287	2292	rVB2	42018	58809	1.94%	0.290%
29	16.210	2365	2367	2373	rVB3	28619	40890	1.35%	0.201%

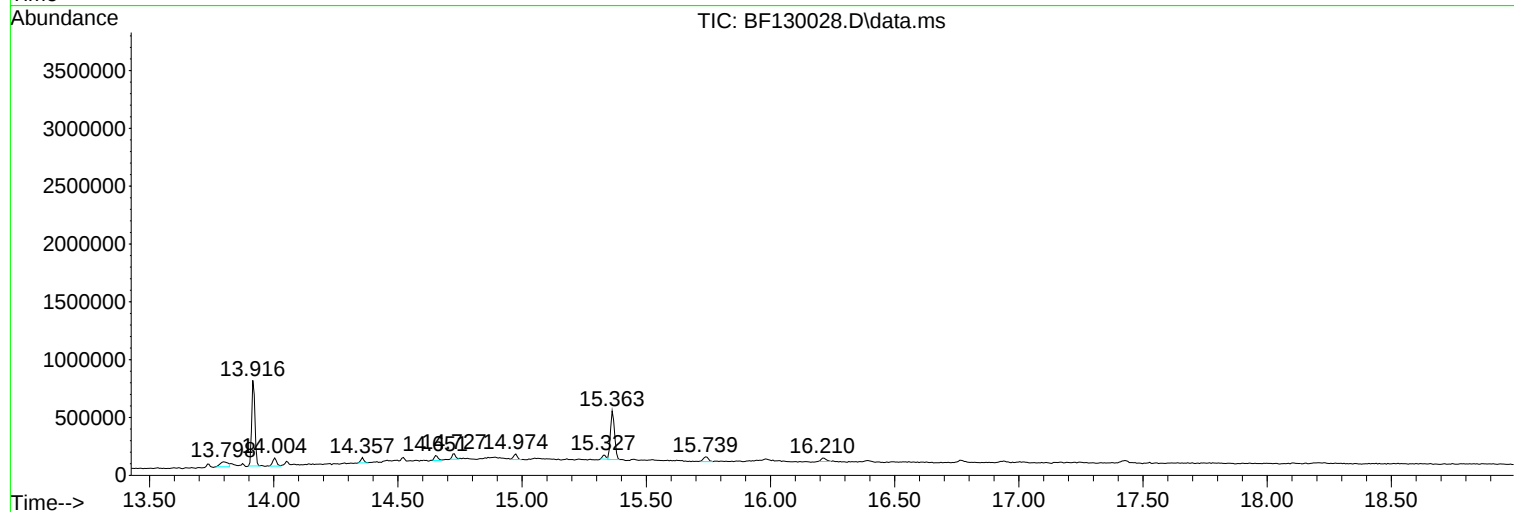
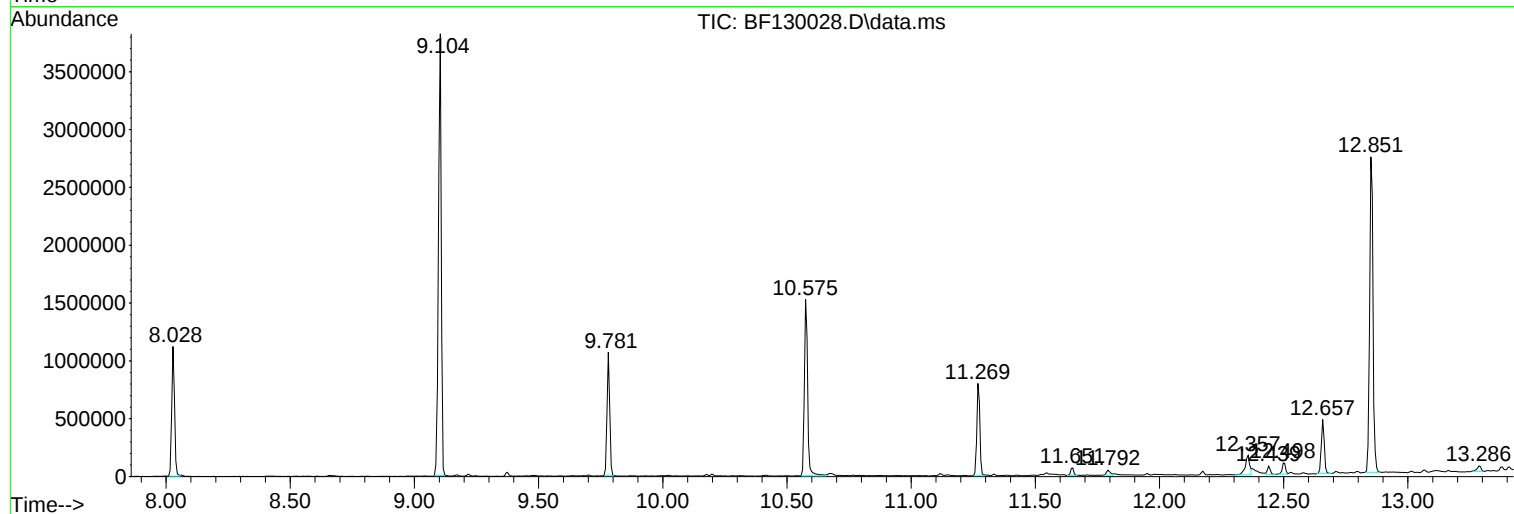
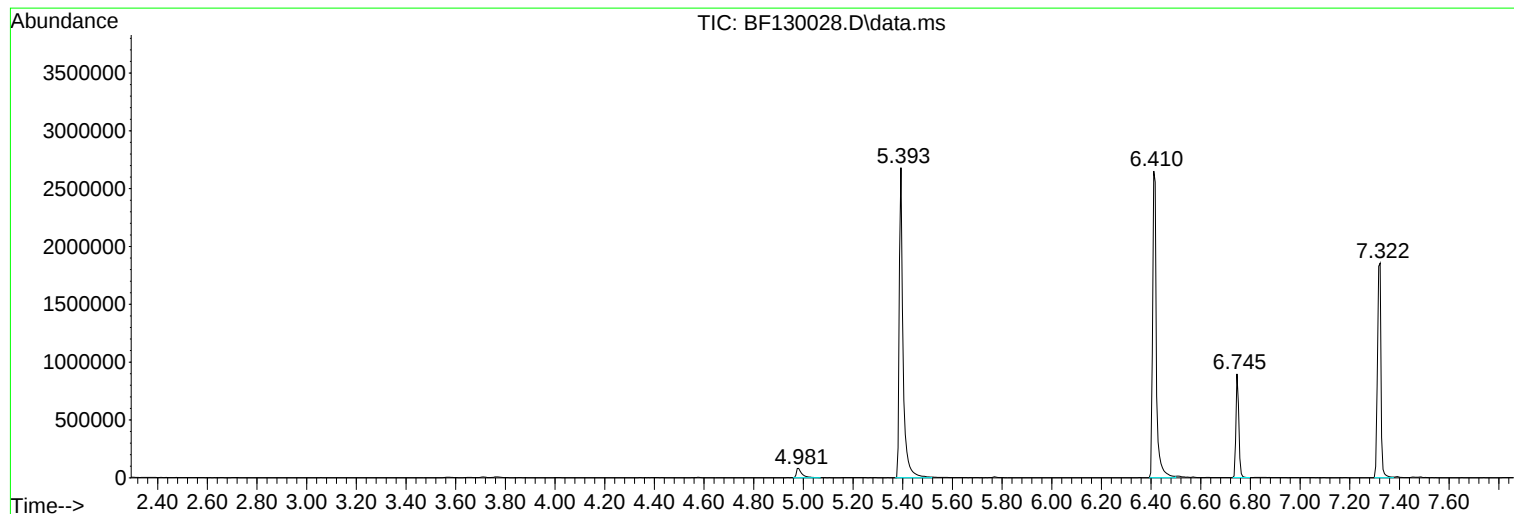
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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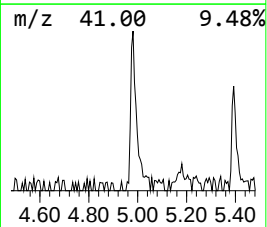
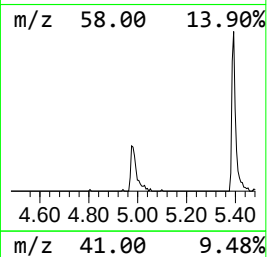
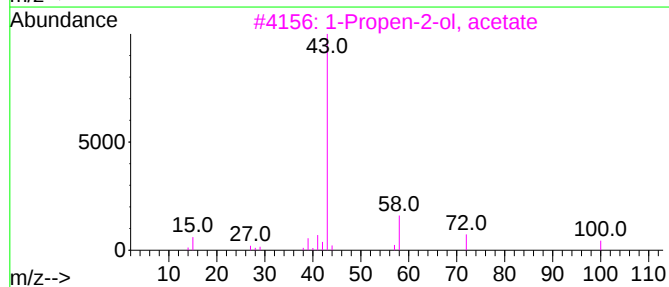
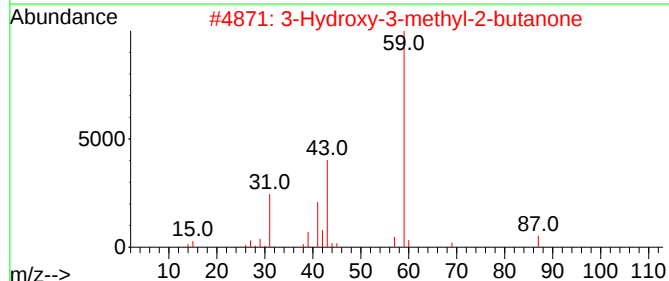
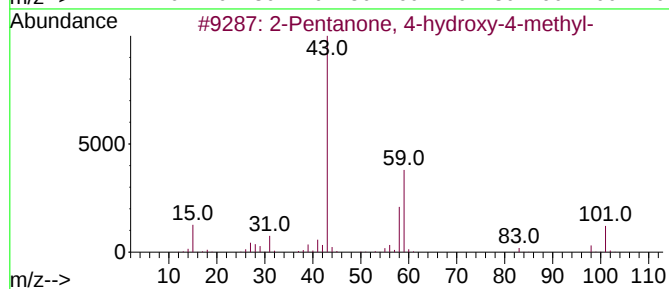
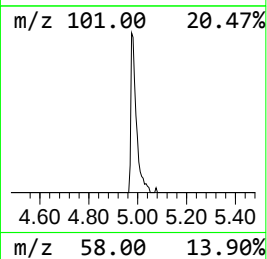
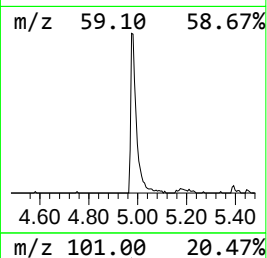
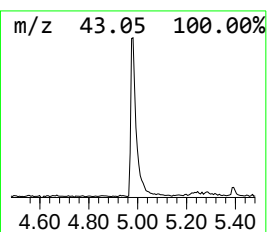
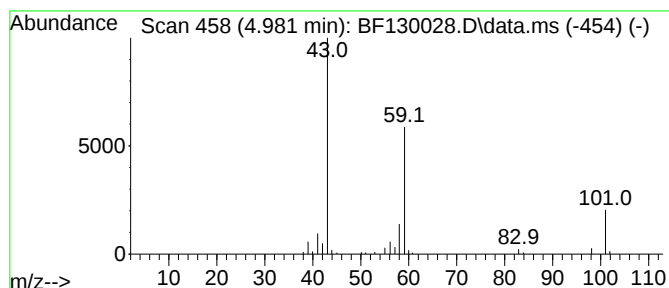
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	3.41 ng	124848	1,4-Dichlorobenzene-d4	6.745

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	



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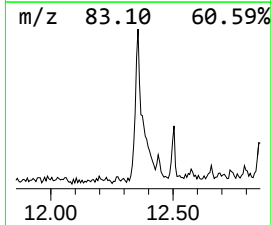
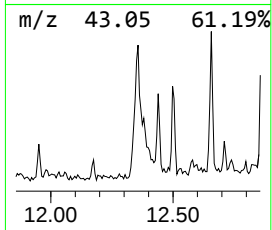
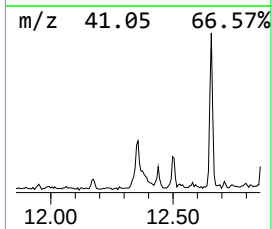
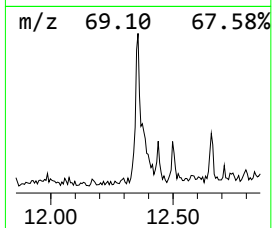
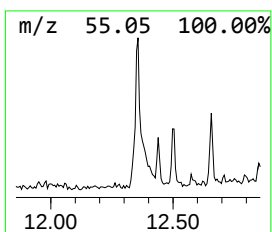
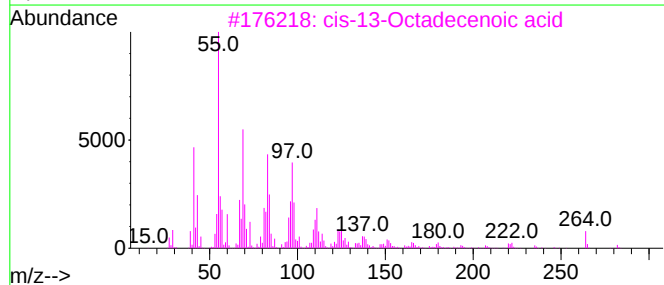
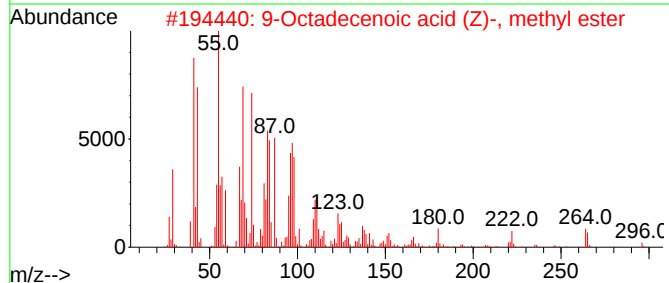
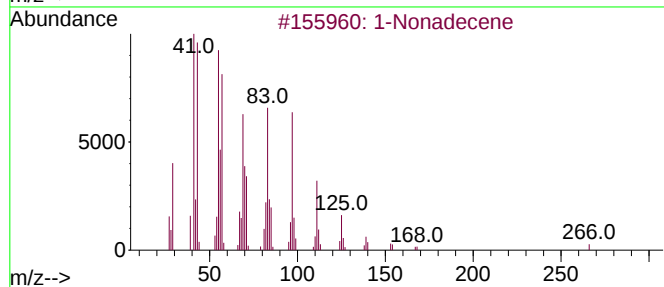
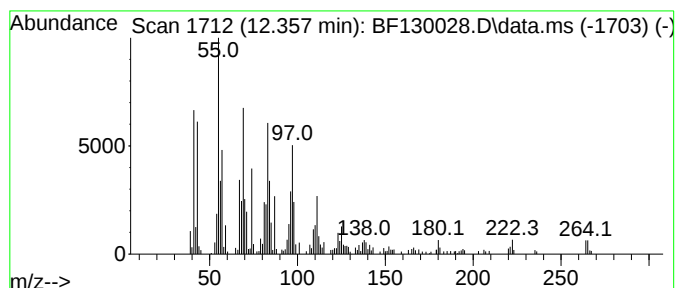
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Peak Number 2 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	6.28 ng	211537	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	93
2	9-Octadecenoic acid (Z)-, methyl...			296	C19H36O2	000112-62-9	76
3	cis-13-Octadecenoic acid			282	C18H34O2	013126-39-1	62
4	9-Octadecenoic acid, (E)-			282	C18H34O2	000112-79-8	58
5	cis-Vaccenic acid			282	C18H34O2	000506-17-2	58



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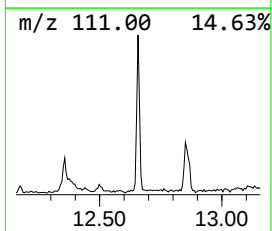
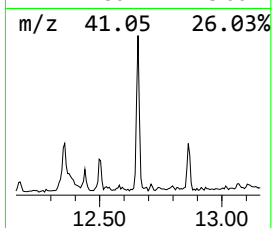
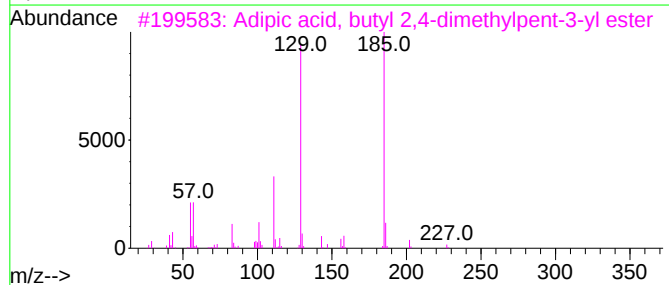
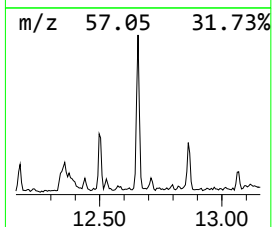
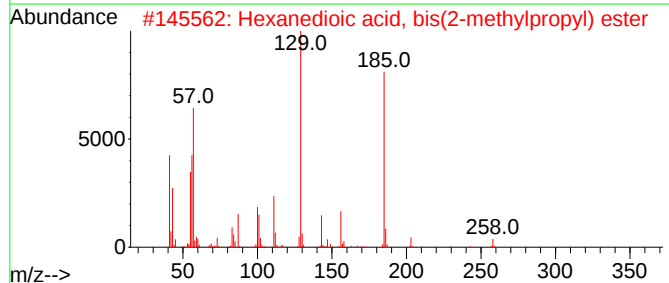
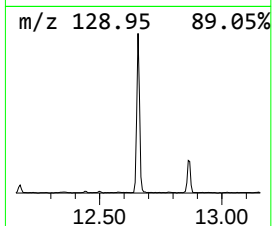
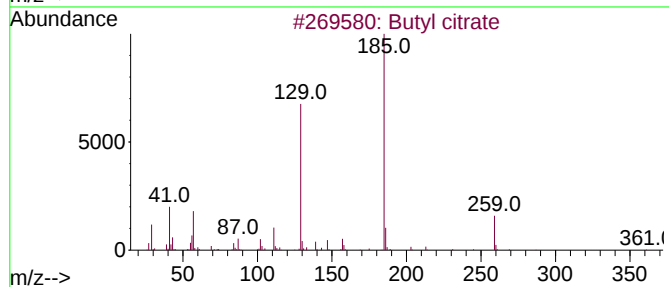
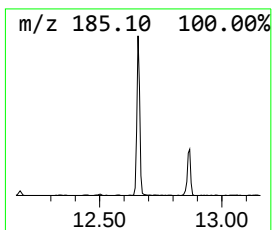
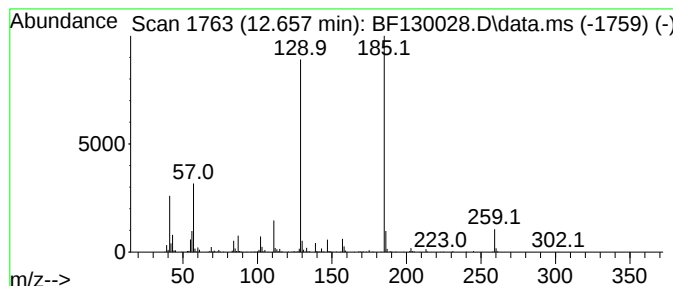
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Peak Number 4 Butyl citrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.657	11.46 ng	381145	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	72
3			Adipic acid, butyl 2,4-dimethylp...	300	C17H32O4	1000349-77-7	72
4			Adipic acid, butyl 2-methylpent-...	286	C16H30O4	1010353-55-8	72
5			Adipic acid, 2-ethylcyclohexyl i...	312	C18H32O4	1000324-22-5	53



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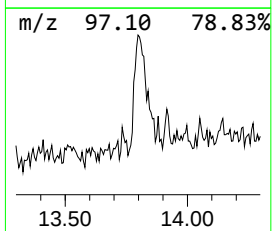
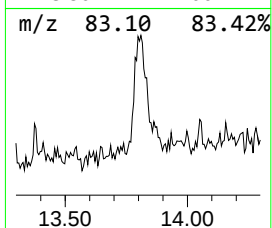
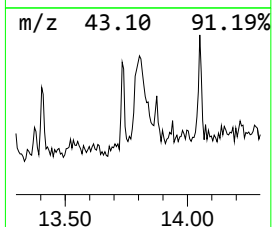
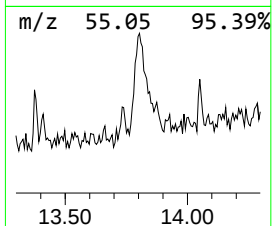
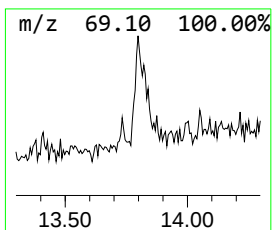
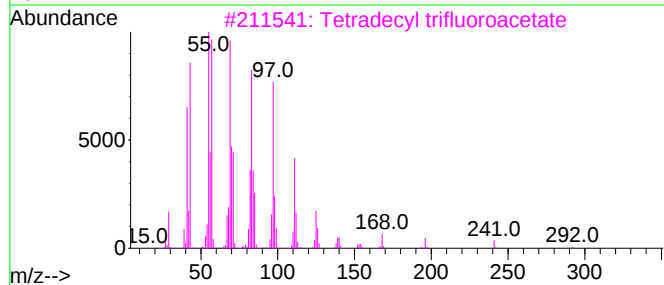
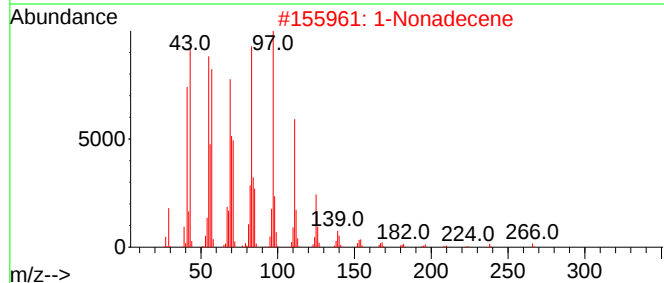
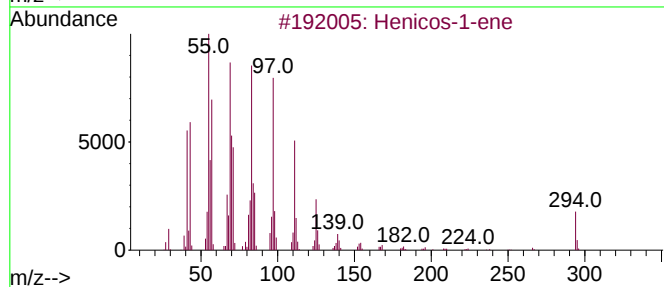
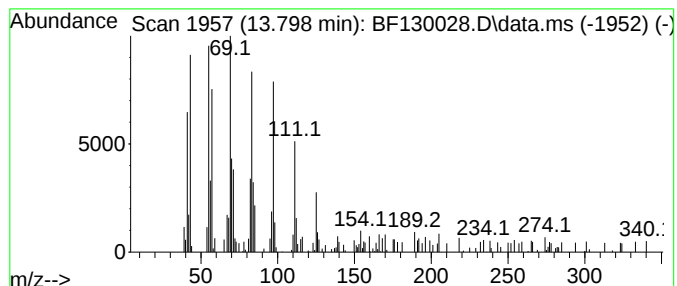
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Peak Number 5 Henicos-1-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.88 ng	95719	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Henicos-1-ene	294	C21H42	001599-68-4	94
2			1-Nonadecene	266	C19H38	018435-45-5	92
3			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
4			3-Heptadecene, (Z)-	238	C17H34	1000141-67-3	91
5			9-Octadecene, (E)-	252	C18H36	007206-25-9	89



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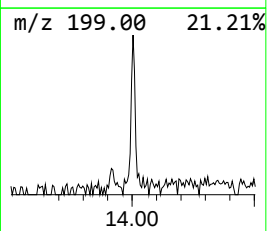
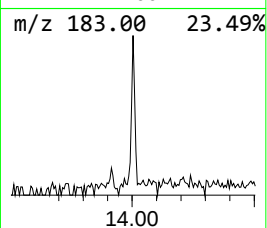
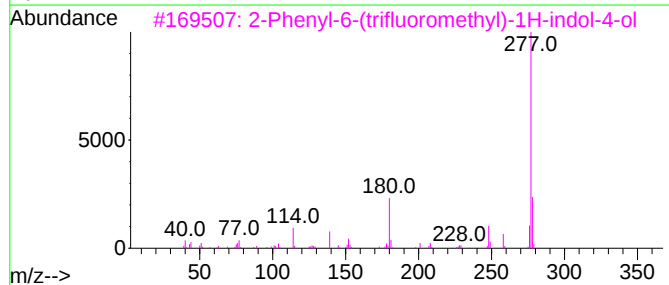
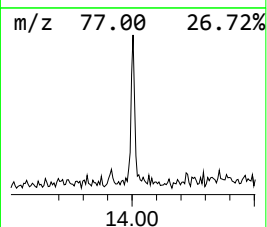
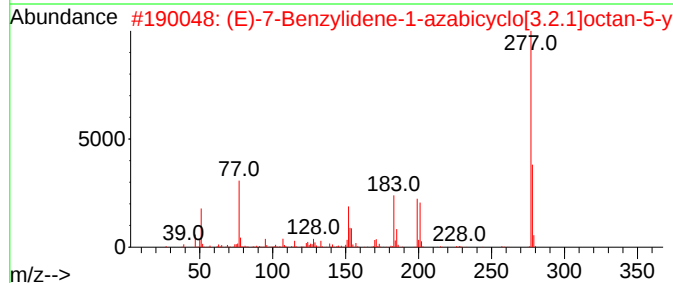
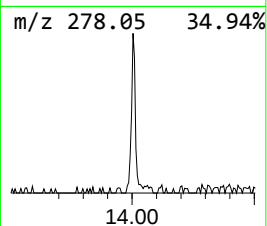
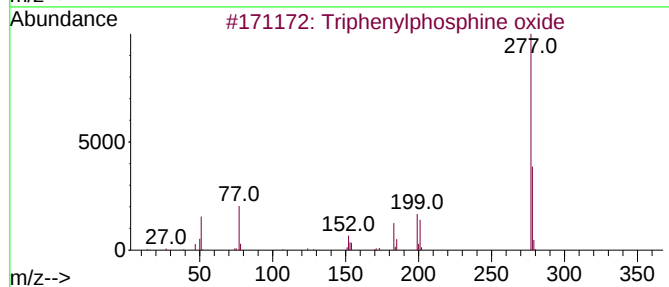
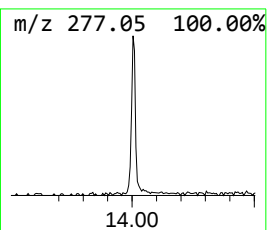
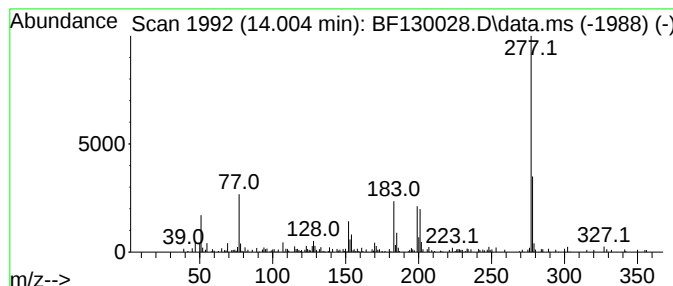
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Peak Number 6 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	2.33 ng	77488	Chrysene-d12	13.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	68
3			2-Phenyl-6-(trifluoromethyl)-1H...	277	C15H10F3NO	1000387-59-3	43
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42



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SB-04-12-13

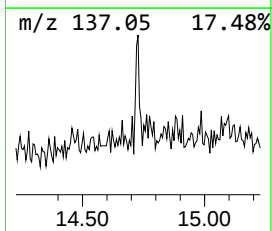
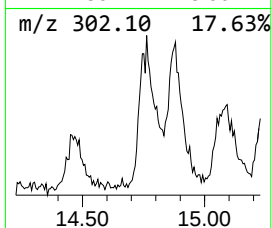
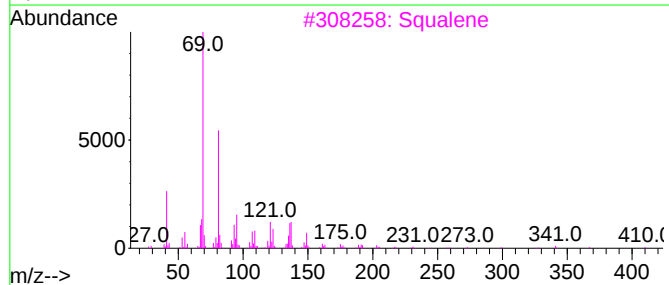
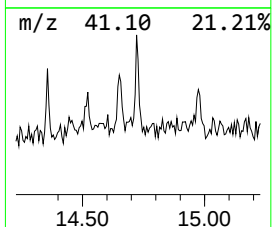
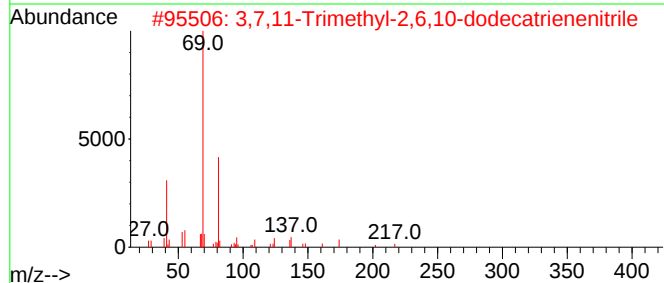
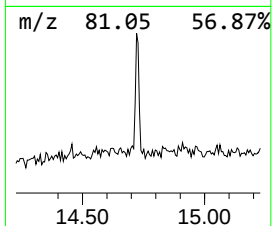
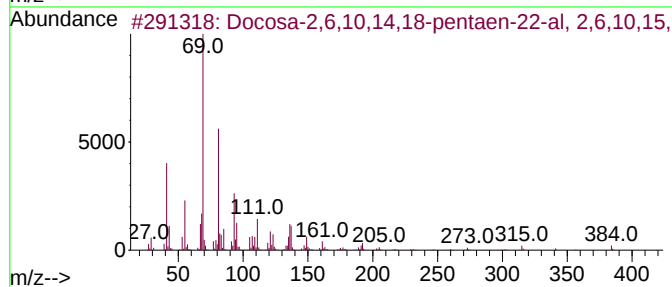
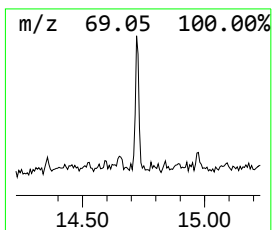
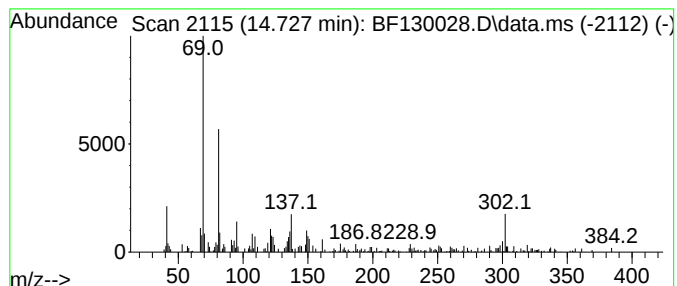
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosa-2,6,10,14,18-pentaen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	2.06 ng	49326	Perylene-d12	15.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	91
2			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	76
3			Squalene	410	C30H50	000111-02-4	72
4			trans-Geranylgeraniol	290	C20H34O	024034-73-9	68
5			Supraene	410	C30H50	007683-64-9	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130028.D
Acq On : 26 Aug 2022 20:19
Operator : CG\JU
Sample : N4379-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-12-13

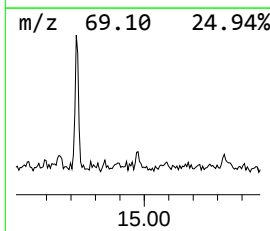
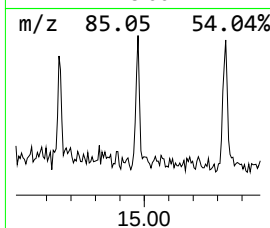
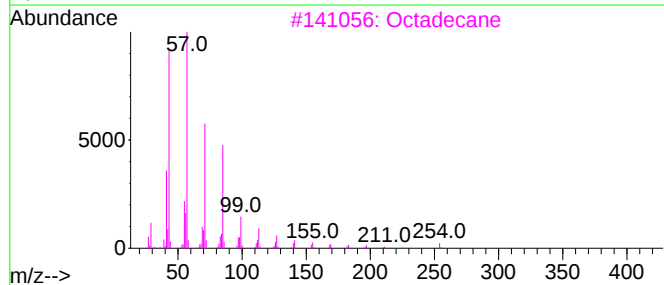
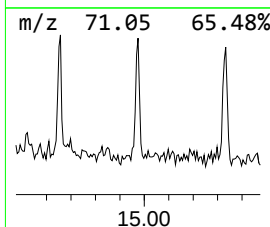
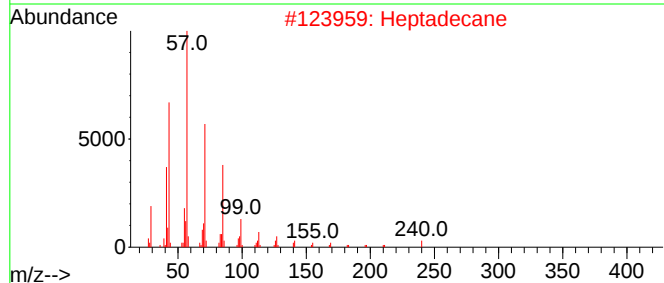
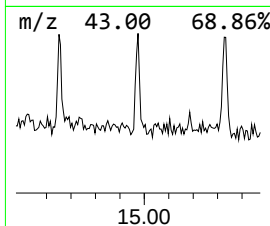
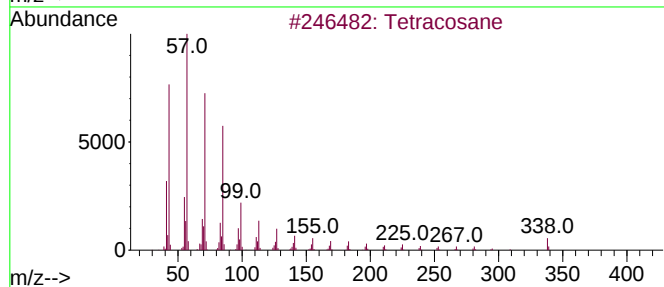
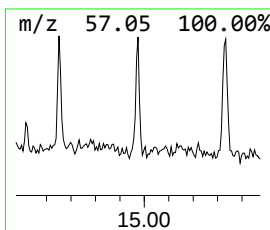
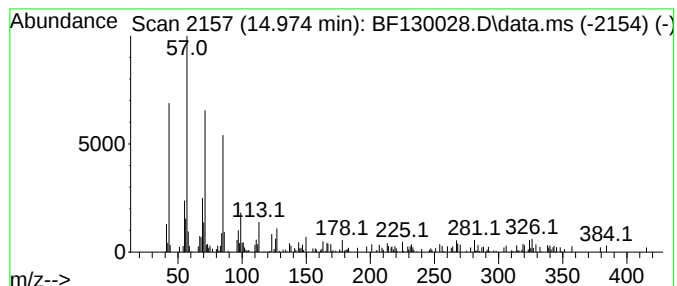
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	2.03 ng	48678	Perylene-d12	15.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Heptadecane	240	C17H36	000629-78-7	86
3			Octadecane	254	C18H38	000593-45-3	86
4			Nonadecane	268	C19H40	000629-92-5	86
5			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130028.D
Acq On : 26 Aug 2022 20:19
Operator : CG\JU
Sample : N4379-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-12-13

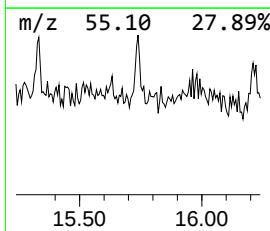
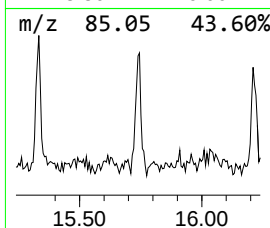
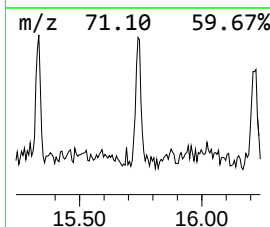
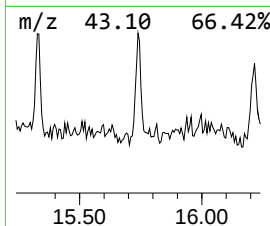
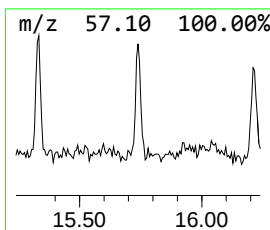
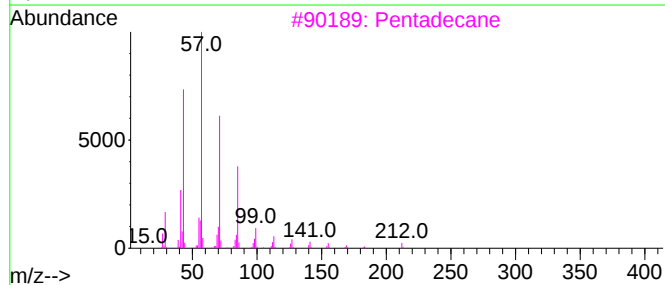
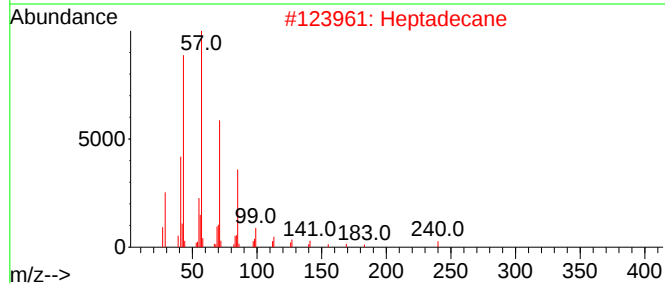
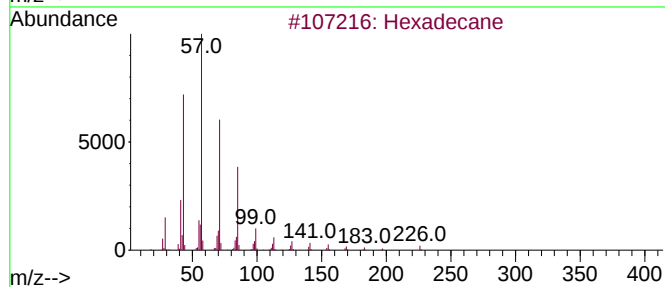
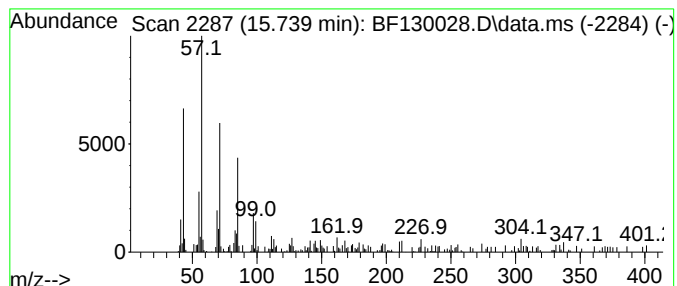
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	2.46 ng	58809	Perylene-d12	15.363

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane	226	C16H34	000544-76-3	89
2		Heptadecane	240	C17H36	000629-78-7	89
3		Pentadecane	212	C15H32	000629-62-9	81
4		Octadecane	254	C18H38	000593-45-3	76
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130028.D
Acq On : 26 Aug 2022 20:19
Operator : CG\JU
Sample : N4379-08
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-12-13

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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
2-Pentanone, 4-...	4.981	3.4	ng	124848	1	6.745	731856	20.0
1-Nonadecene	12.357	6.3	ng	211537	4	11.269	674213	20.0
Butyl citrate	12.657	11.5	ng	381145	5	13.916	665319	20.0
Henicos-1-ene	13.798	2.9	ng	95719	5	13.916	665319	20.0
Triphenylphosph...	14.004	2.3	ng	77488	5	13.916	665319	20.0
Docosa-2,6,10,1...	14.727	2.1	ng	49326	6	15.363	478637	20.0
Tetracosane	14.974	2.0	ng	48678	6	15.363	478637	20.0
Hexadecane	15.739	2.5	ng	58809	6	15.363	478637	20.0