

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
 Data File : BF142029.D
 Acq On : 21 Mar 2025 14:52
 Operator : RC/JU
 Sample : Q1619-05
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF031025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142029.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	21	rVB	853145	1369360	41.11%	5.509%
2	4.475	399	405	412	rBV	159863	239757	7.20%	0.965%
3	5.093	499	510	518	rBV2	71833	121231	3.64%	0.488%
4	5.493	571	578	587	rBV	1830597	2539613	76.24%	10.218%
5	6.492	742	748	767	rBV	1930977	2789493	83.75%	11.223%
6	6.875	808	813	819	rBV	655850	816610	24.52%	3.286%
7	7.434	902	908	918	rBV	1133738	1520699	45.65%	6.118%
8	7.686	946	951	961	rBV	50015	69112	2.07%	0.278%
9	8.157	1025	1031	1047	rBV	795002	1117219	33.54%	4.495%
10	8.369	1063	1067	1076	rBV	26630	39120	1.17%	0.157%
11	9.228	1207	1213	1223	rBV	2664741	3330897	100.00%	13.401%
12	9.910	1323	1329	1339	rVB	980293	1263747	37.94%	5.085%
13	10.210	1374	1380	1394	rBV	17127	56052	1.68%	0.226%
14	10.622	1444	1450	1457	rBV	241818	316245	9.49%	1.272%
15	10.692	1457	1462	1479	rVV	1548573	2092837	62.83%	8.420%
16	11.392	1576	1581	1597	rBV	908806	1222472	36.70%	4.918%
17	11.916	1664	1670	1682	rBV2	133286	264671	7.95%	1.065%
18	12.169	1710	1713	1720	rVB3	22576	33853	1.02%	0.136%
19	12.610	1784	1788	1791	rBV	45696	61995	1.86%	0.249%
20	12.704	1798	1804	1821	rBV	175680	372667	11.19%	1.499%
21	12.833	1822	1826	1832	rVB	40872	66738	2.00%	0.269%
22	12.980	1845	1851	1856	rBV	2326437	2999441	90.05%	12.068%
23	13.874	1998	2003	2014	rBV	94899	182866	5.49%	0.736%
24	14.033	2024	2030	2040	rVB	580826	827939	24.86%	3.331%
25	14.504	2106	2110	2114	rBV3	28084	49750	1.49%	0.200%
26	14.886	2170	2175	2182	rVB	131060	192325	5.77%	0.774%
27	15.074	2204	2207	2215	rVB	29827	57265	1.72%	0.230%
28	15.504	2275	2280	2293	rVB	487582	840888	25.25%	3.383%

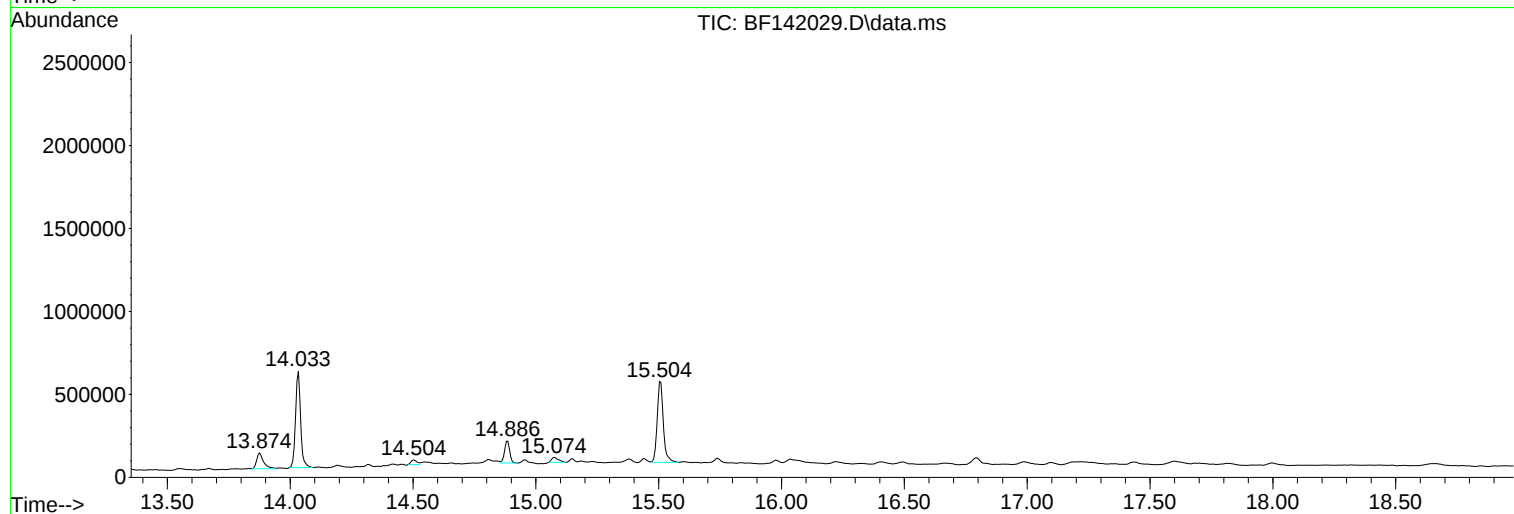
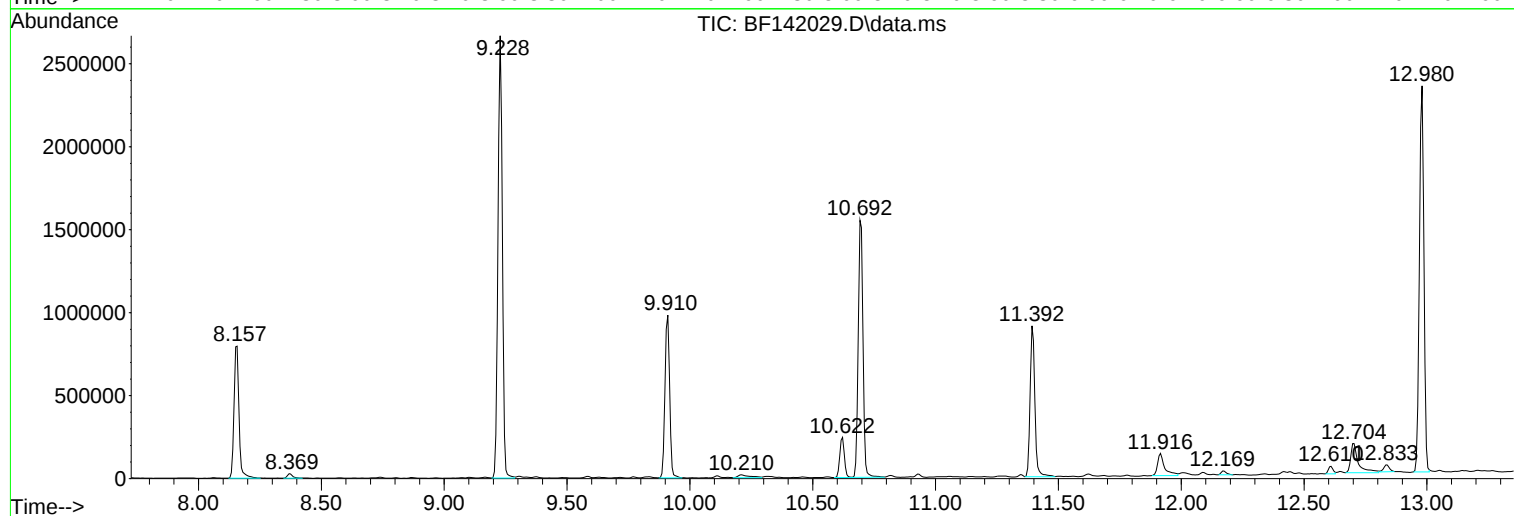
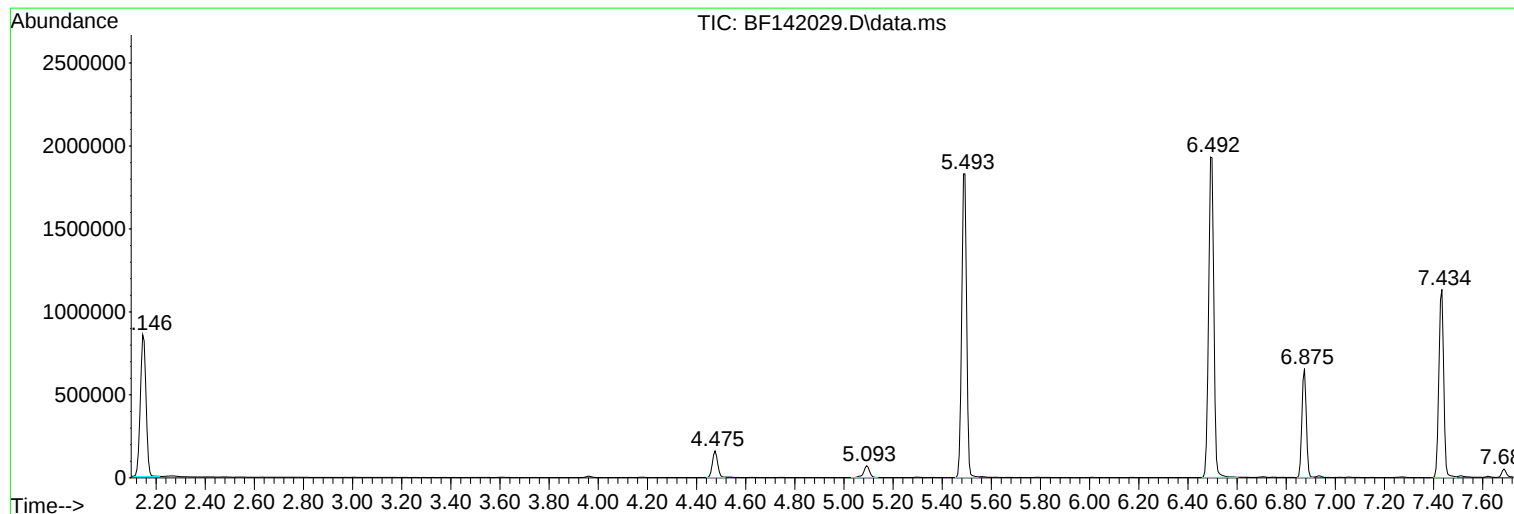
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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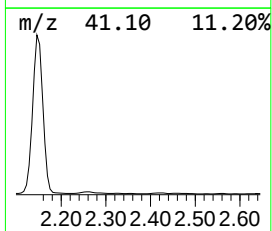
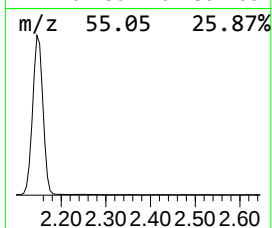
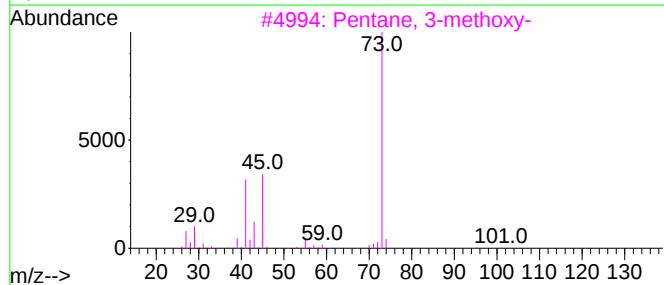
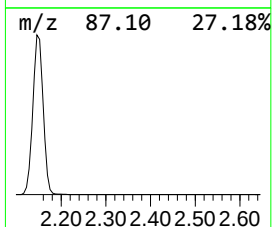
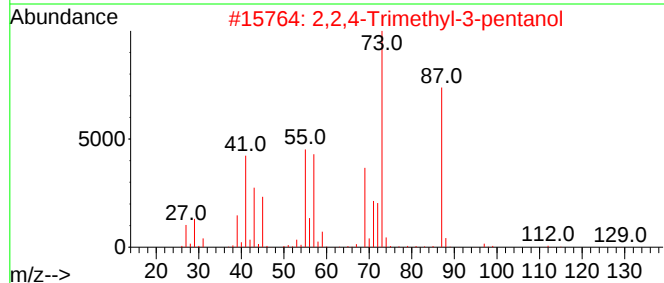
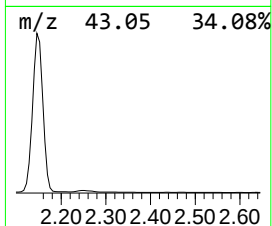
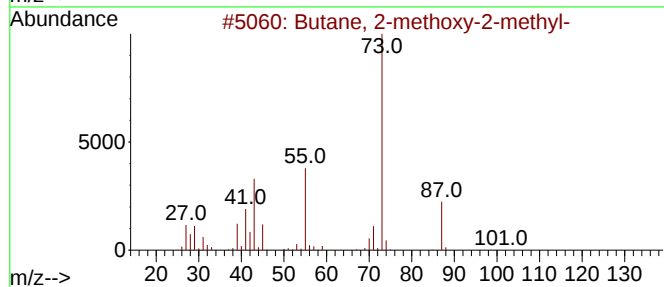
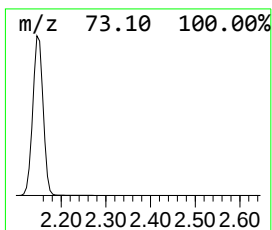
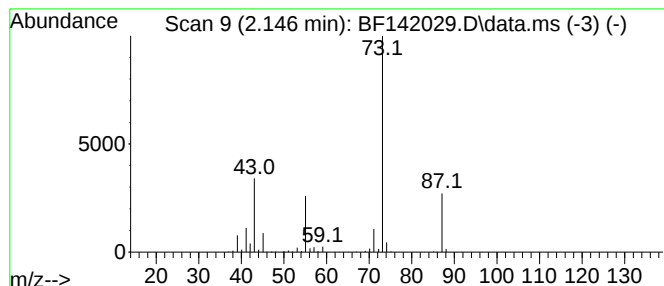
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	33.54 ng	1369360	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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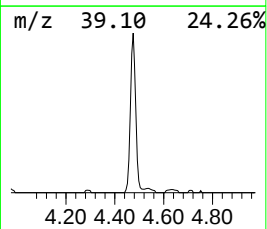
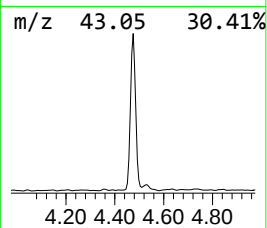
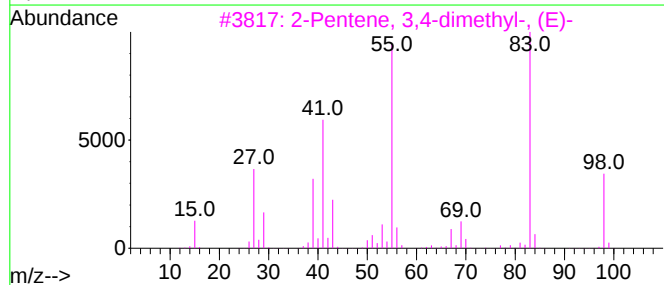
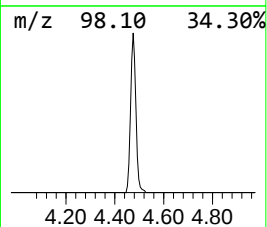
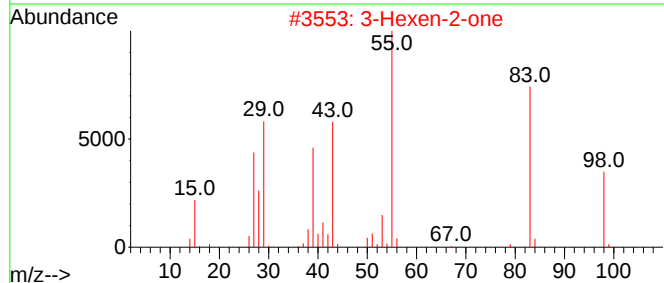
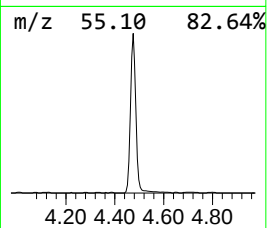
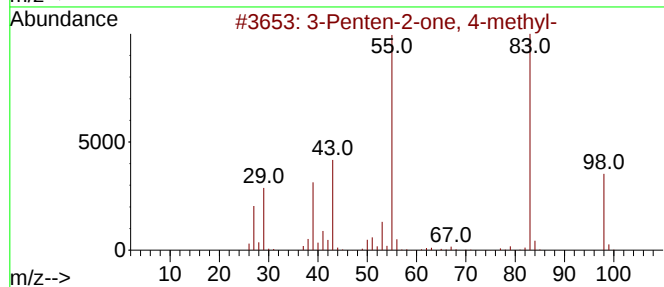
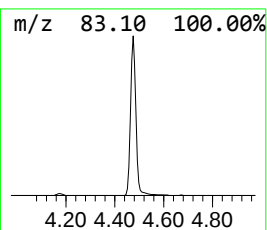
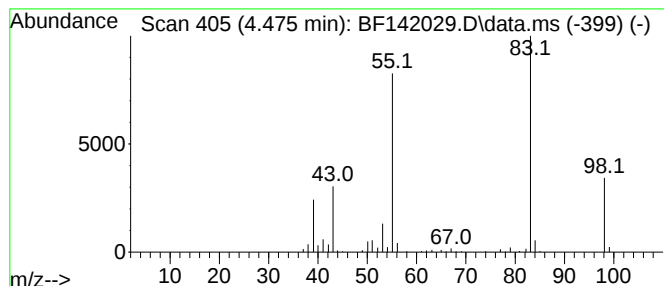
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	5.87 ng	239757	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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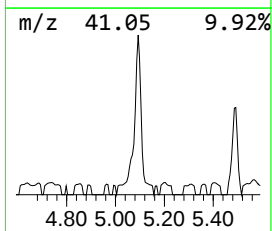
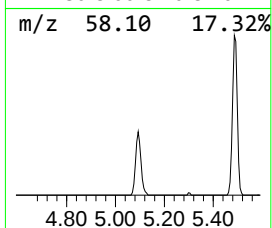
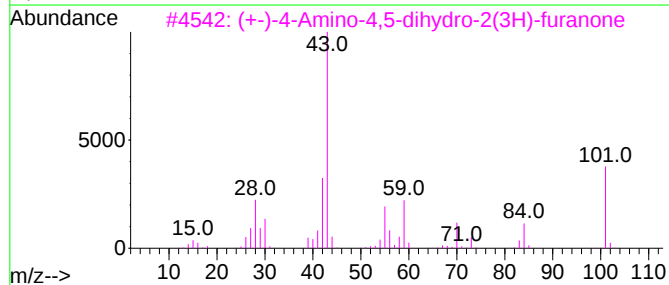
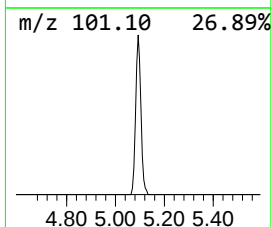
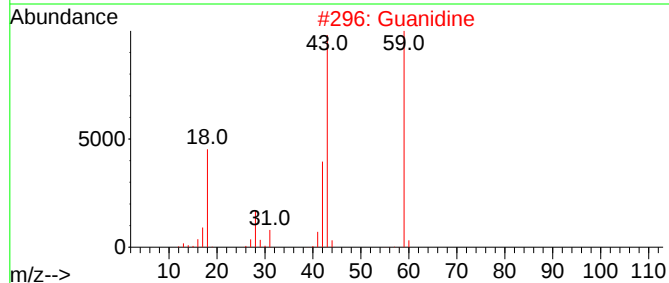
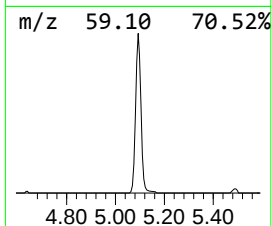
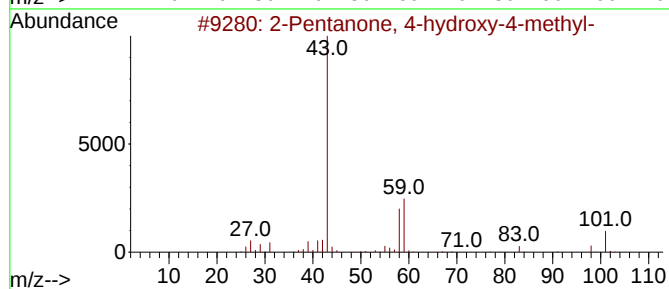
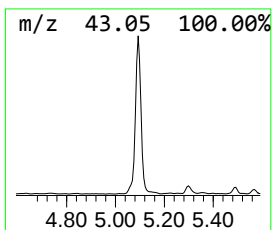
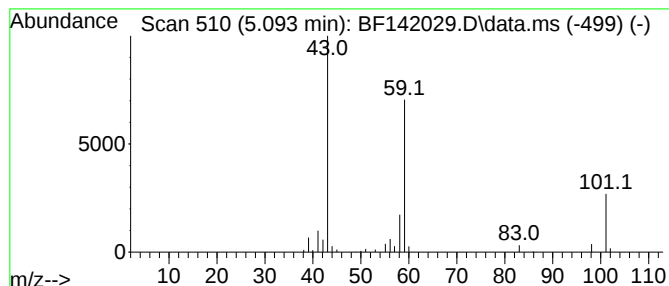
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.97 ng	121231	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Guanidine	59	CH5N3	000113-00-8	43
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17



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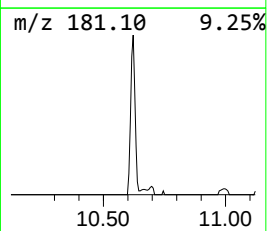
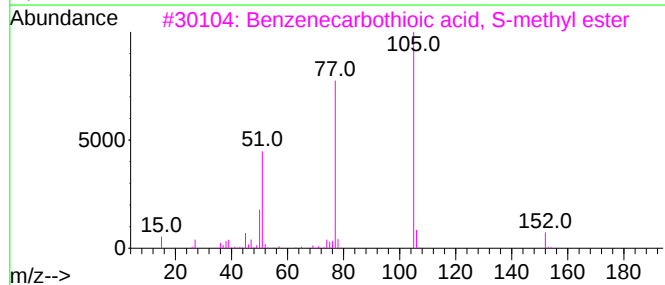
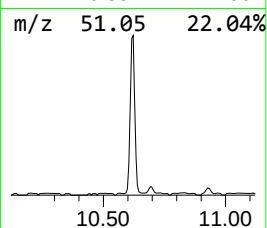
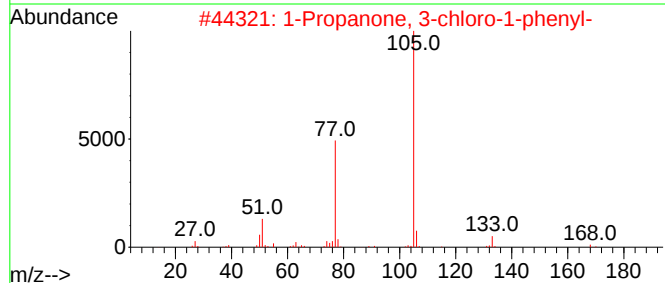
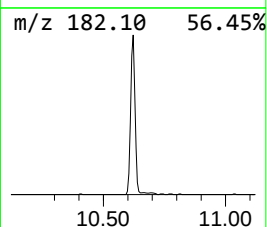
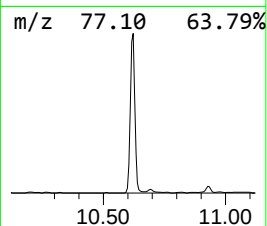
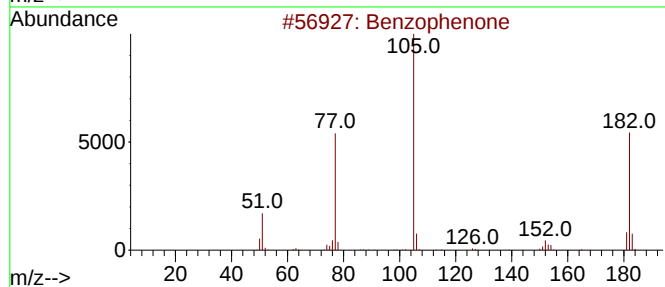
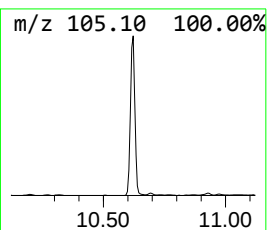
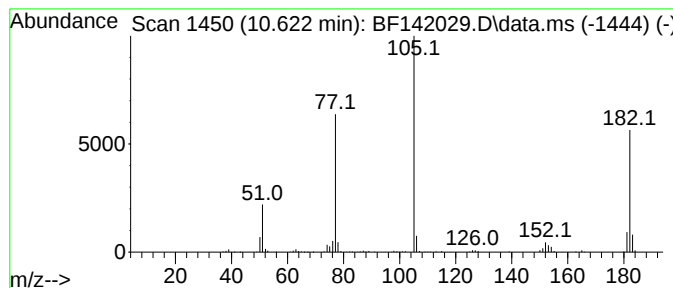
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	5.00 ng	316245	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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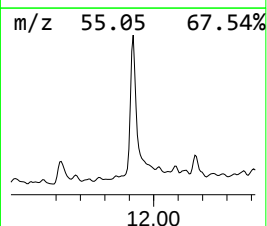
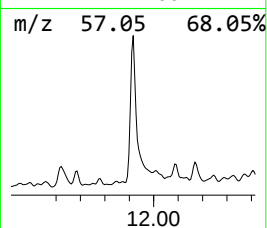
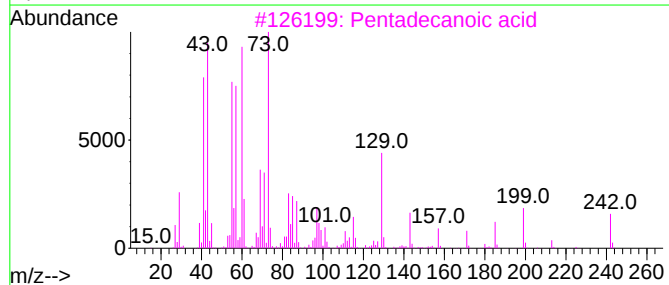
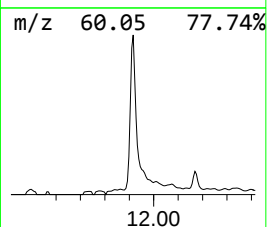
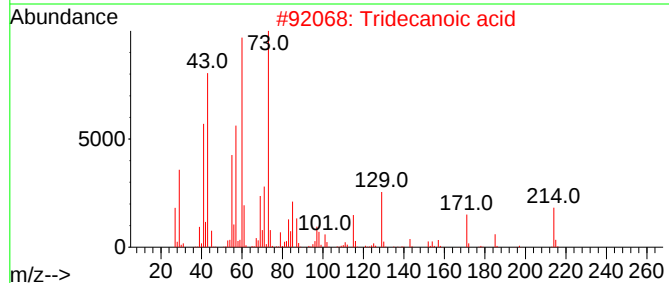
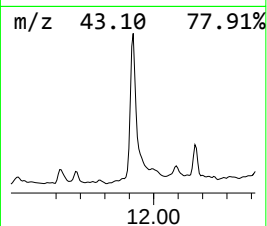
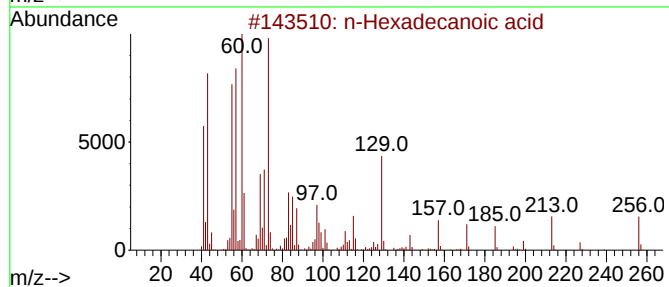
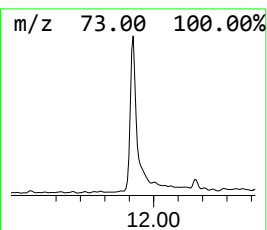
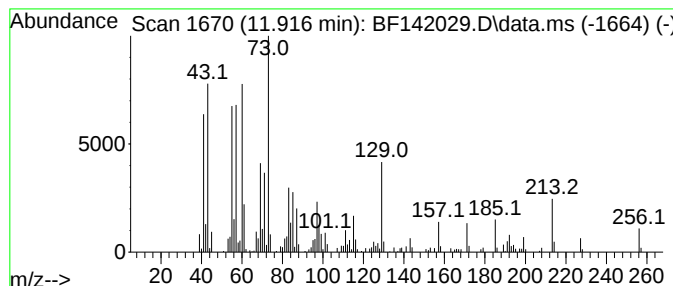
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.33 ng	264671	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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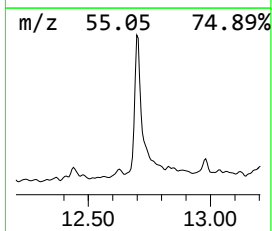
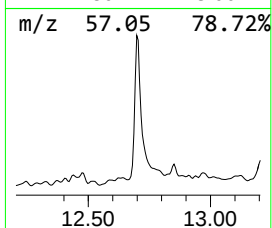
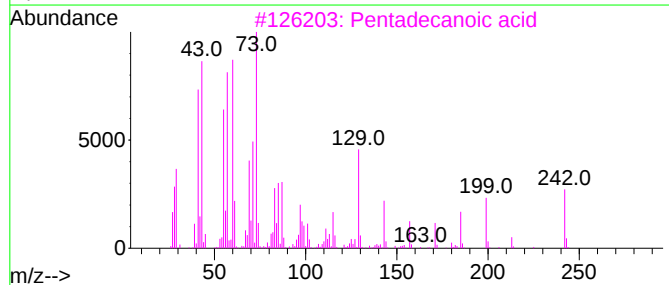
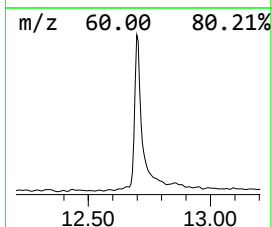
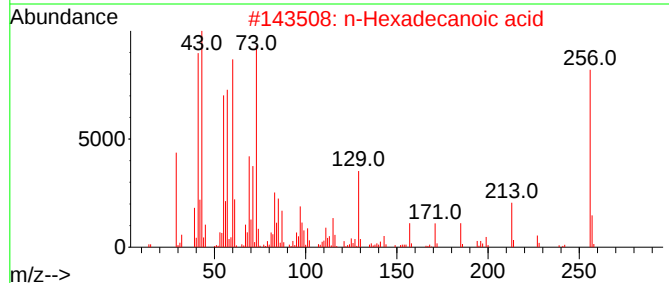
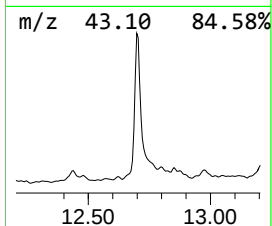
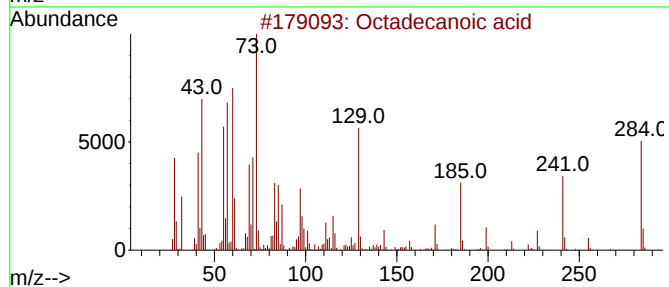
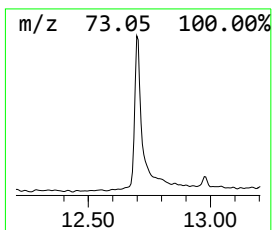
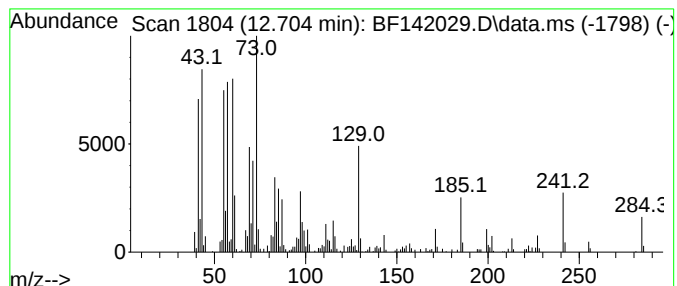
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	6.10 ng	372667	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
Data File : BF142029.D
Acq On : 21 Mar 2025 14:52
Operator : RC/JU
Sample : Q1619-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

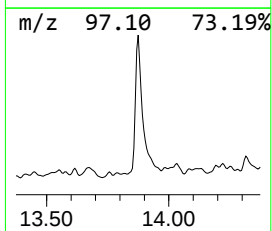
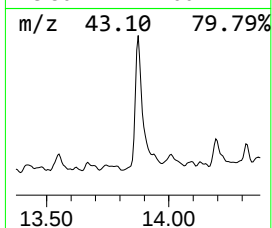
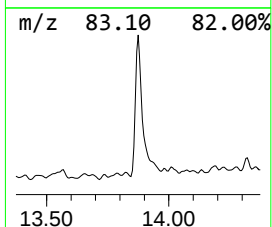
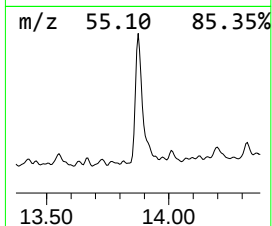
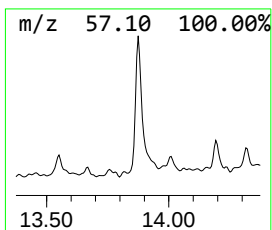
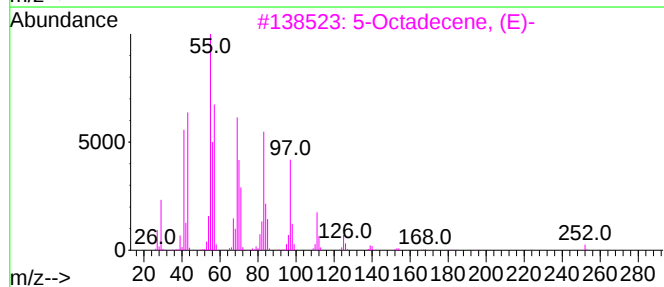
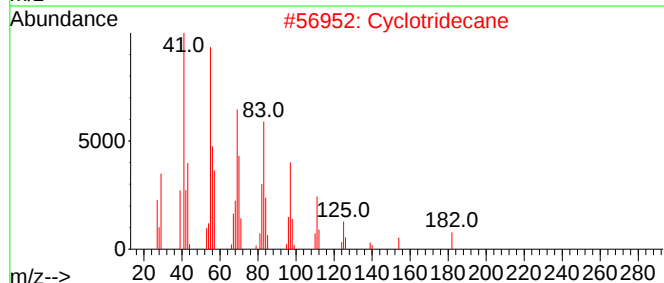
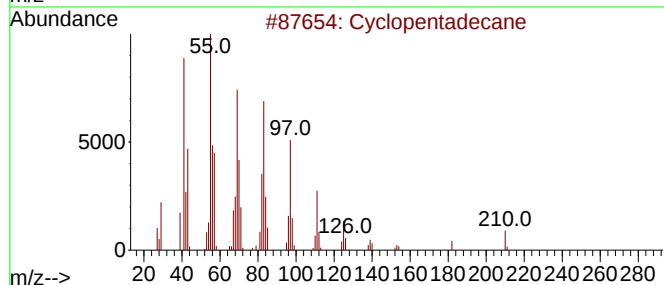
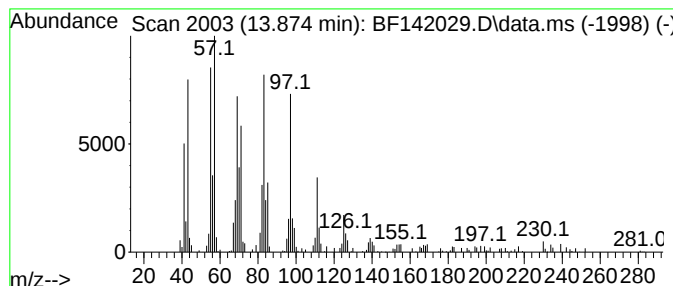
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	4.42 ng	182866	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	98
2			Cyclotridecane	182	C13H26	000295-02-3	97
3			5-Octadecene, (E)-	252	C18H36	007206-21-5	95
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
Data File : BF142029.D
Acq On : 21 Mar 2025 14:52
Operator : RC/JU
Sample : Q1619-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

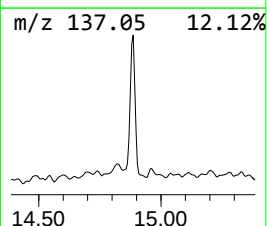
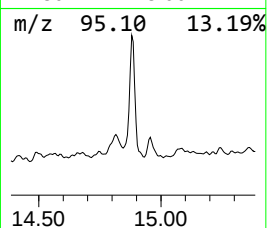
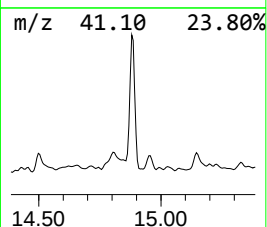
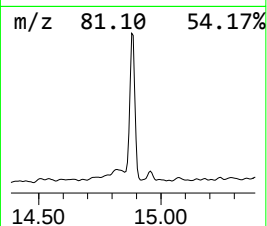
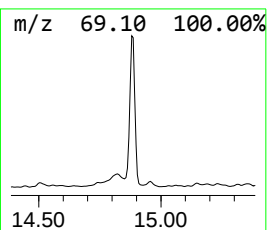
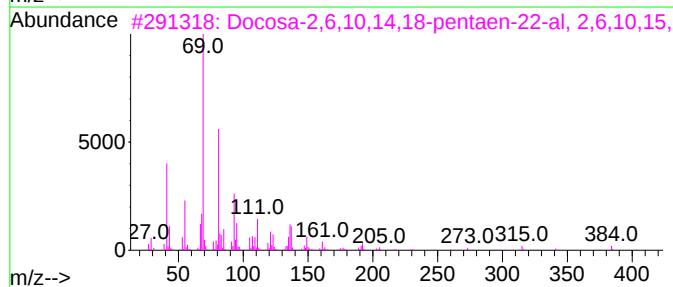
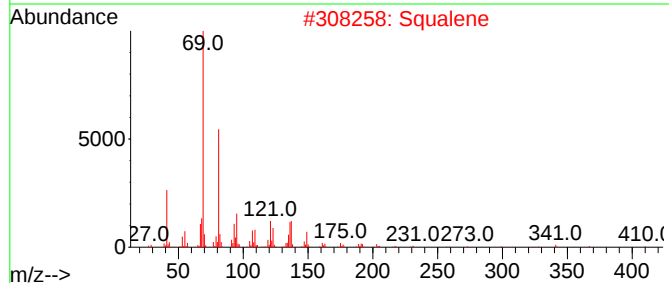
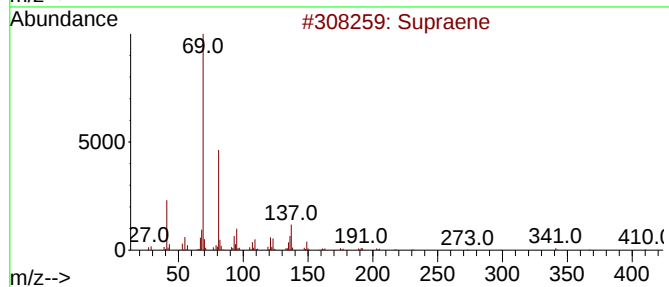
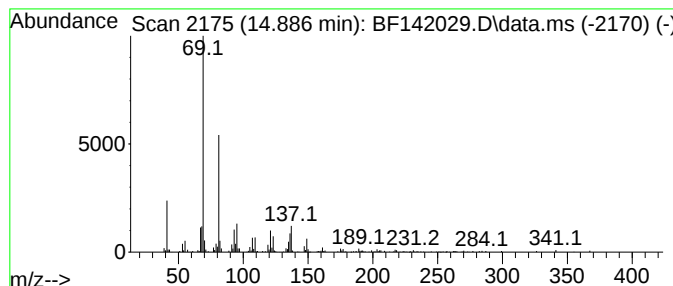
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	4.57 ng	192325	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5			trans-Farnesol	222	C15H26O	000106-28-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
Data File : BF142029.D
Acq On : 21 Mar 2025 14:52
Operator : RC/JU
Sample : Q1619-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	33.5	ng	1369360	1	6.875	816610	20.0
3-Penten-2-one,...	4.475	5.9	ng	239757	1	6.875	816610	20.0
2-Pentanone, 4-...	5.093	3.0	ng	121231	1	6.875	816610	20.0
Benzophenone	10.622	5.0	ng	316245	3	9.910	1263750	20.0
n-Hexadecanoic ...	11.916	4.3	ng	264671	4	11.392	1222470	20.0
Octadecanoic acid	12.704	6.1	ng	372667	4	11.392	1222470	20.0
Cyclopentadecane	13.874	4.4	ng	182866	5	14.033	827939	20.0
Supraene	14.886	4.6	ng	192325	6	15.504	840888	20.0