

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030625\
 Data File : BF141866.D
 Acq On : 06 Mar 2025 14:01
 Operator : RC/JU
 Sample : Q1489-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2

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-BF022725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141866.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	5	12	19	rBV	1017691	1600998	42.08%	4.291%
2	5.110	502	513	521	rBV2	25570	53221	1.40%	0.143%
3	5.498	573	579	584	rBV	2513545	3288377	86.43%	8.814%
4	6.498	743	749	766	rBV	2493473	3426773	90.07%	9.185%
5	6.887	809	815	820	rVB	736304	949273	24.95%	2.544%
6	7.439	903	909	914	rBV	1642651	2105717	55.35%	5.644%
7	7.692	947	952	958	rVB	79713	96206	2.53%	0.258%
8	8.163	1027	1032	1040	rBV	1009273	1368400	35.97%	3.668%
9	8.375	1062	1068	1076	rVB3	41203	62522	1.64%	0.168%
10	8.875	1147	1153	1159	rBV	40786	50621	1.33%	0.136%
11	9.239	1209	1215	1220	rBV	2896293	3804527	100.00%	10.197%
12	9.775	1302	1306	1312	rVB	45346	57957	1.52%	0.155%
13	9.916	1324	1330	1334	rBV	1145693	1431476	37.63%	3.837%
14	9.945	1334	1335	1340	rVB	49648	47340	1.24%	0.127%
15	10.116	1358	1364	1369	rBV	56709	82380	2.17%	0.221%
16	10.463	1419	1423	1429	rVB	146548	182772	4.80%	0.490%
17	10.627	1446	1451	1458	rBV	289223	366365	9.63%	0.982%
18	10.704	1458	1464	1477	rBV	2010323	2665642	70.07%	7.145%
19	11.010	1508	1516	1519	rBV2	35820	63236	1.66%	0.169%
20	11.298	1561	1565	1571	rVB	44227	62188	1.63%	0.167%
21	11.404	1577	1583	1585	rBV	1098055	1545206	40.61%	4.142%
22	11.474	1591	1595	1599	rBV	217387	255688	6.72%	0.685%
23	11.627	1615	1621	1629	rBV2	65434	134089	3.52%	0.359%
24	11.927	1664	1672	1678	rBV	917492	1374914	36.14%	3.685%
25	12.016	1683	1687	1695	rVB2	152939	265871	6.99%	0.713%
26	12.198	1715	1718	1725	rVB	54392	74795	1.97%	0.200%
27	12.486	1763	1767	1773	rVB4	64495	115566	3.04%	0.310%
28	12.616	1784	1789	1793	rBV	700363	951405	25.01%	2.550%
29	12.657	1793	1796	1800	rVB2	87849	108713	2.86%	0.291%
30	12.710	1801	1805	1812	rBV	371515	539650	14.18%	1.446%
31	12.839	1820	1827	1833	rBV2	512127	785189	20.64%	2.104%
32	12.986	1847	1852	1859	rVB	2790567	3529021	92.76%	9.459%
33	13.168	1880	1883	1887	rVB	119232	141738	3.73%	0.380%
34	13.233	1891	1894	1898	rVB	93567	121503	3.19%	0.326%
35	13.774	1983	1986	1991	rBV2	70422	136263	3.58%	0.365%
36	13.886	2001	2005	2014	rVB2	280441	471751	12.40%	1.264%

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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-BF022725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.033	2025	2030	2044	rBV2	1022906	1870253	49.16%	5.013%
38	15.080	2203	2208	2217	rBV	241829	554691	14.58%	1.487%
39	15.380	2256	2259	2265	rVB	145148	215734	5.67%	0.578%
40	15.445	2266	2270	2275	rVV	189486	285098	7.49%	0.764%
41	15.509	2276	2281	2293	rVB	717403	1300884	34.19%	3.487%
42	16.992	2529	2533	2541	rVB2	83422	164392	4.32%	0.441%
43	18.192	2731	2737	2752	rVB3	216223	601598	15.81%	1.612%

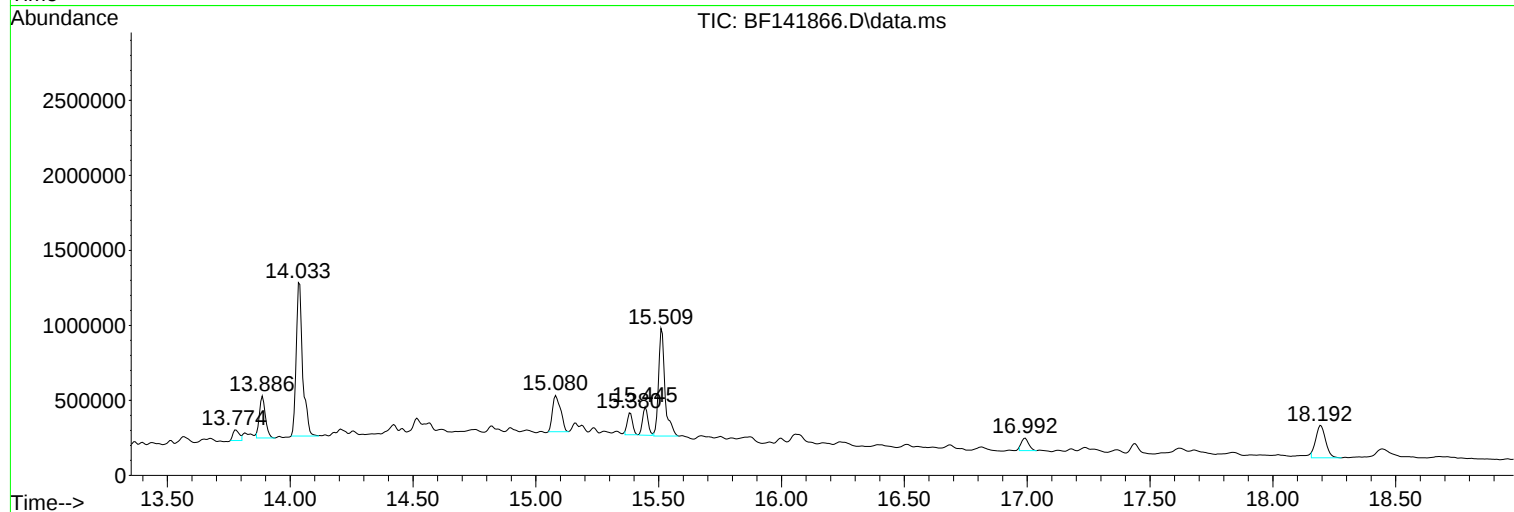
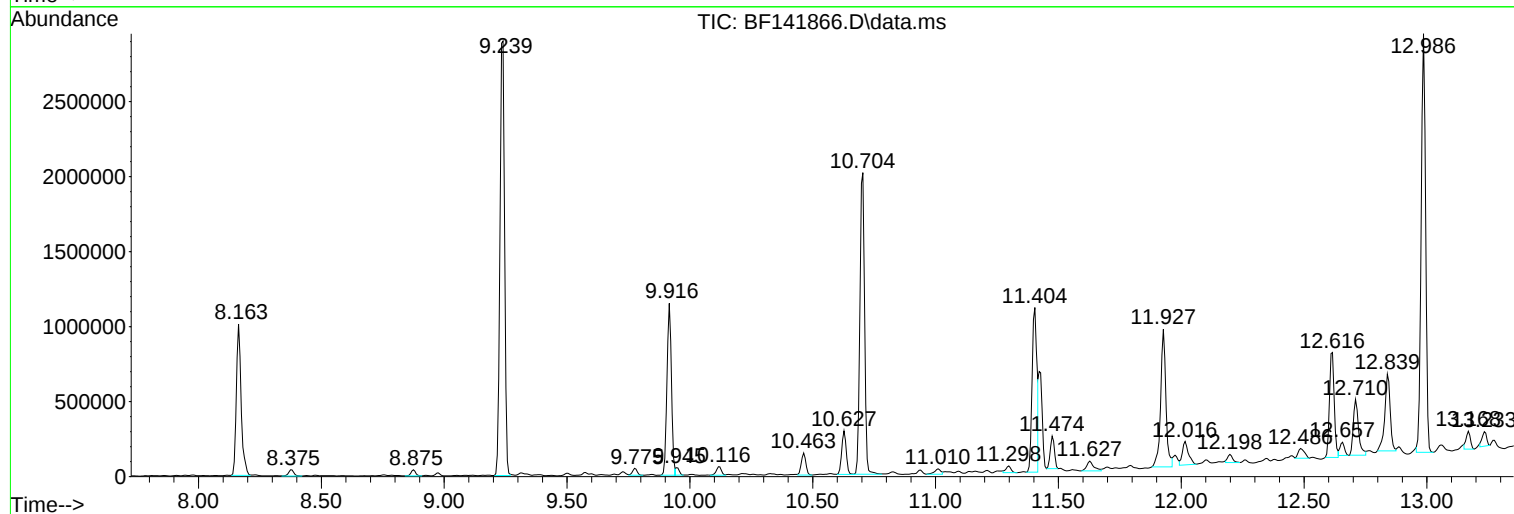
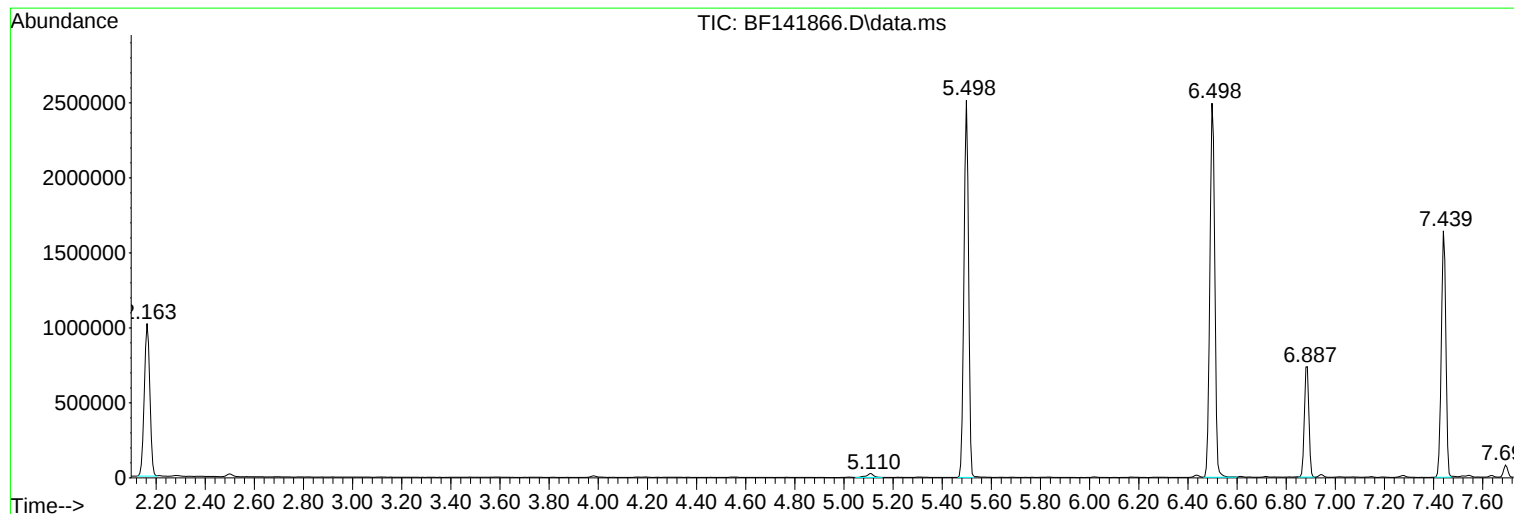
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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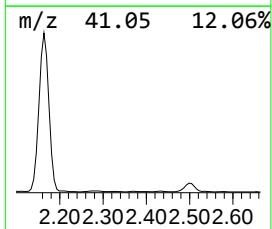
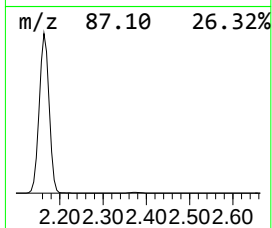
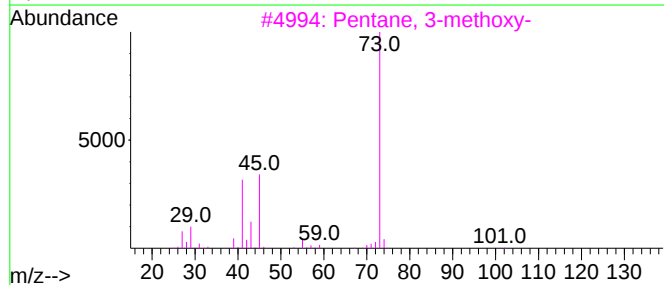
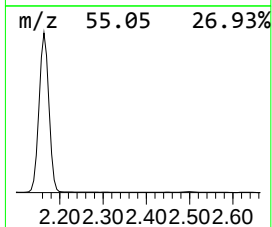
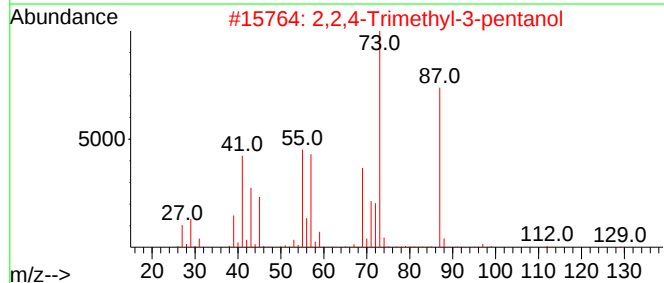
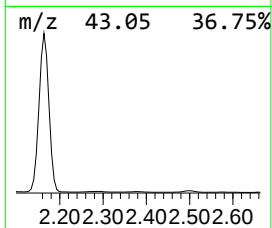
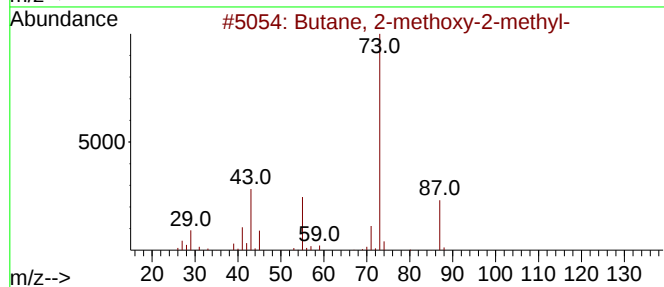
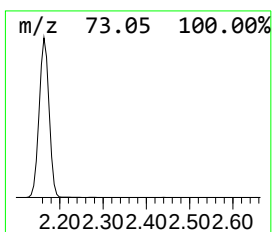
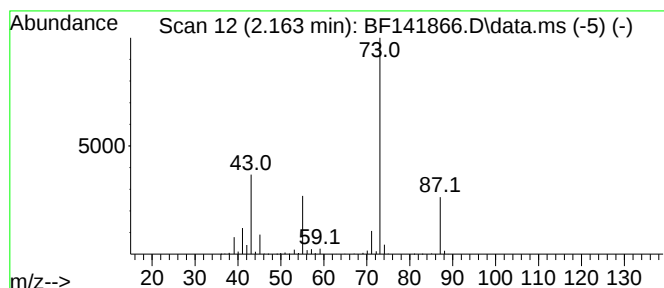
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
2.163	33.73 ng	1601000	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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Misc :
ALS Vial : 10 Sample Multiplier: 1

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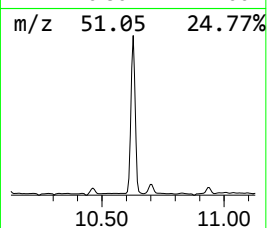
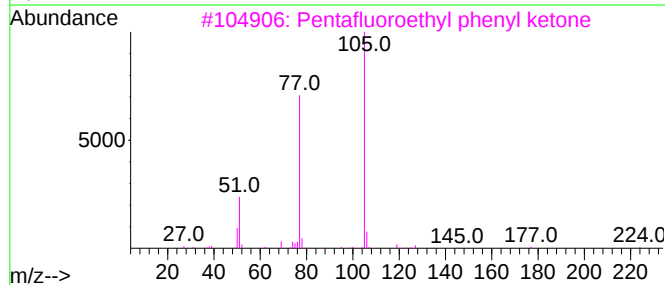
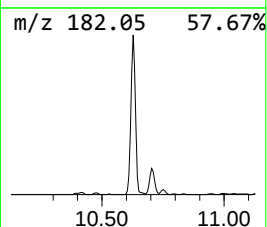
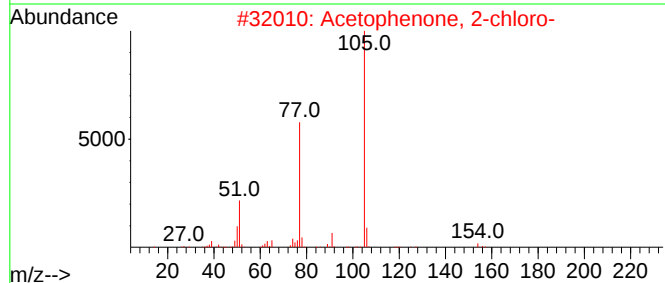
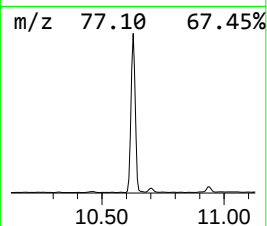
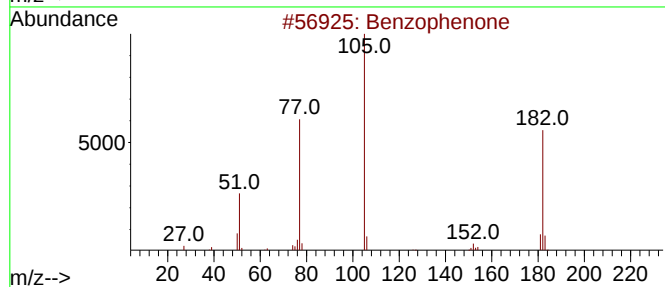
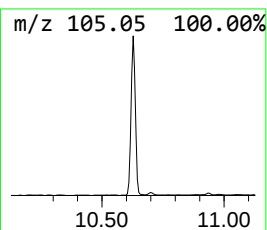
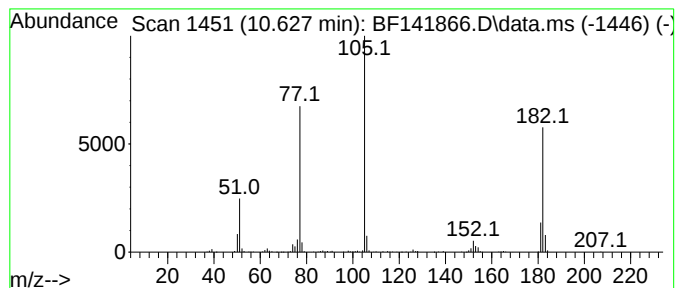
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.627	5.12 ng	366365	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
3			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47



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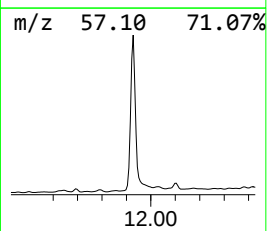
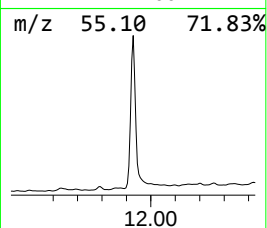
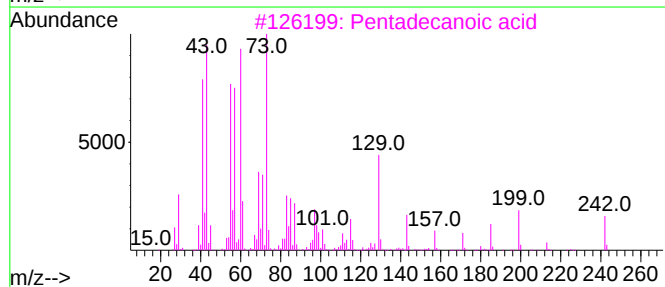
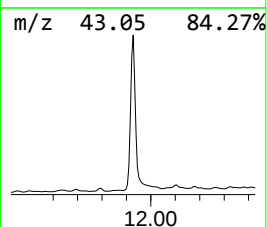
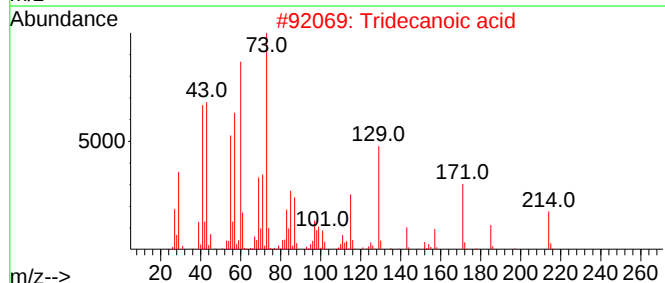
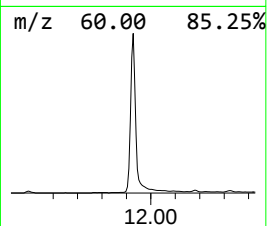
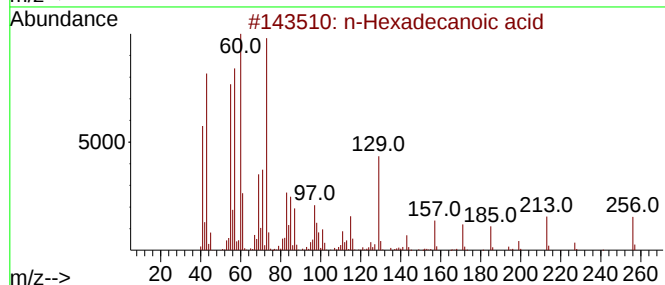
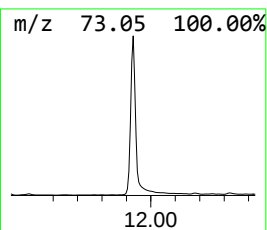
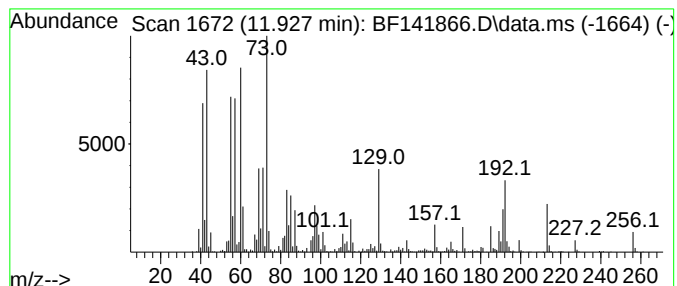
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.927	17.80 ng	1374910	Phenanthrene-d10	11.404	
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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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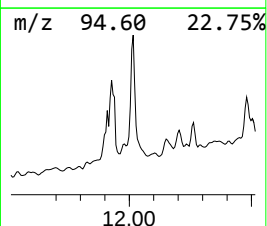
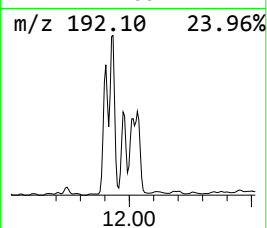
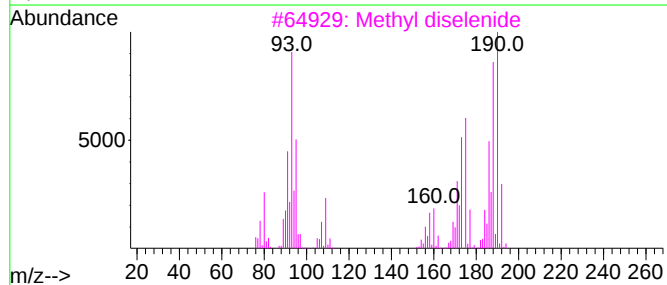
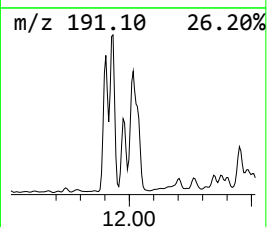
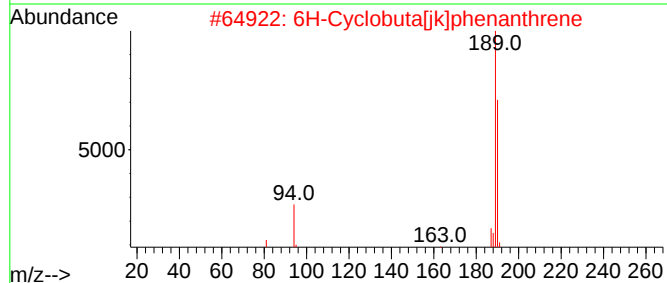
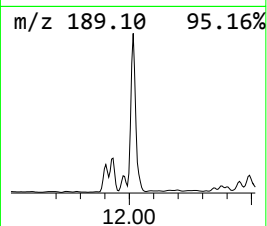
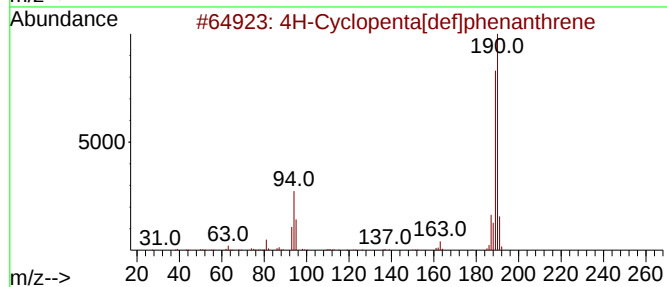
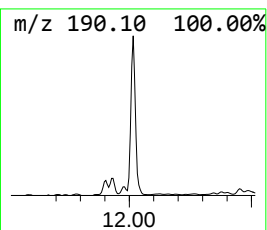
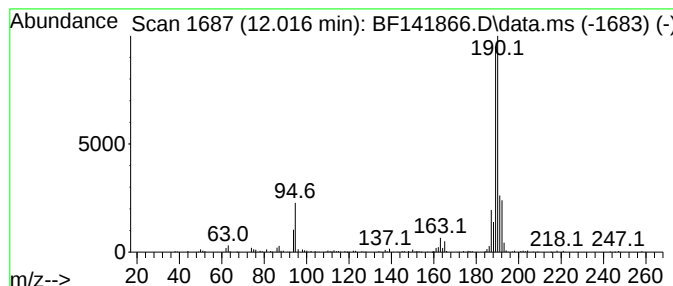
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	3.44 ng	265871	Phenanthrene-d10	11.404

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2		6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3		Methyl diselenide	190	C2H6Se2	007101-31-7	49
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5		1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25



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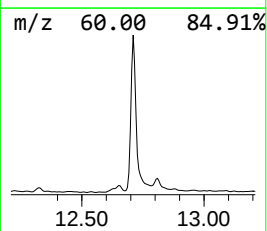
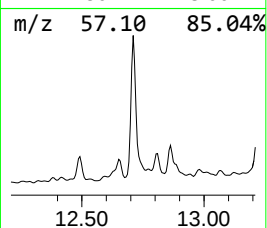
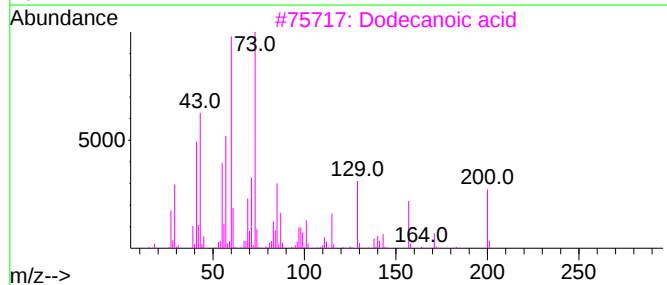
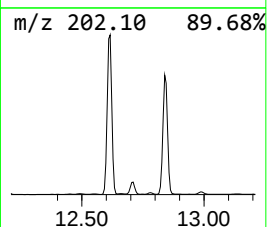
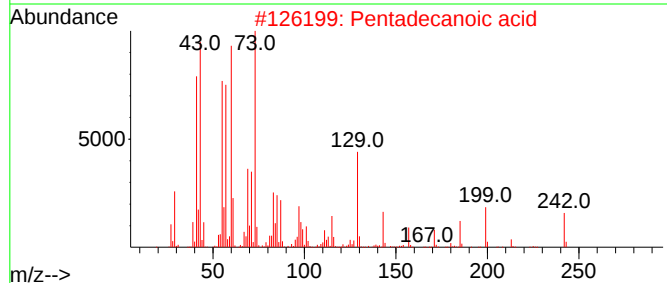
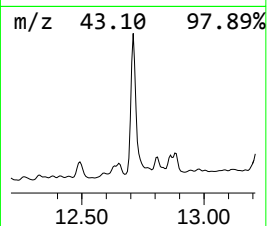
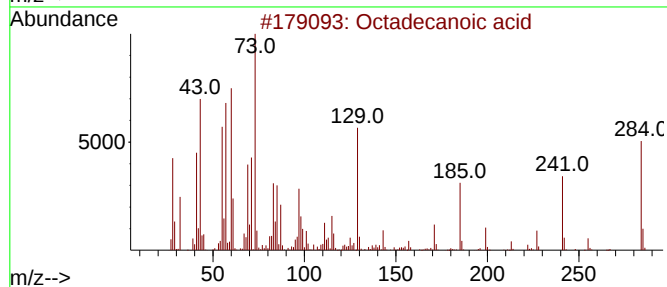
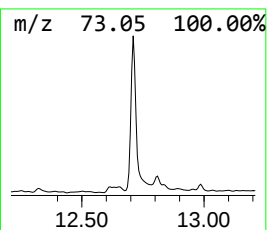
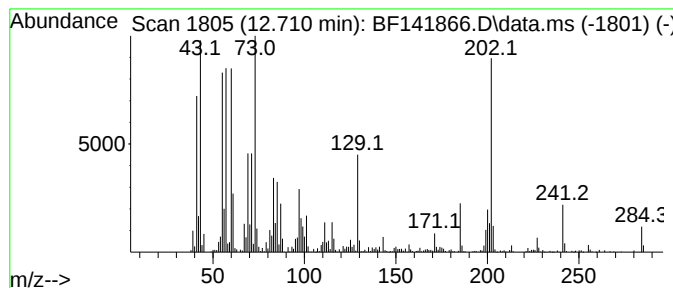
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	6.98 ng	539650	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Dodecanoic acid	200	C12H24O2	000143-07-7	55
4			Fluoranthene	202	C16H10	000206-44-0	53
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030625\
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Acq On : 06 Mar 2025 14:01
Operator : RC/JU
Sample : Q1489-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

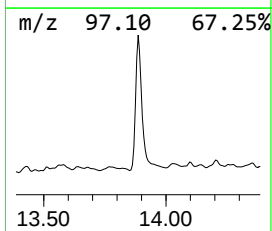
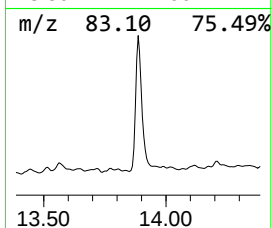
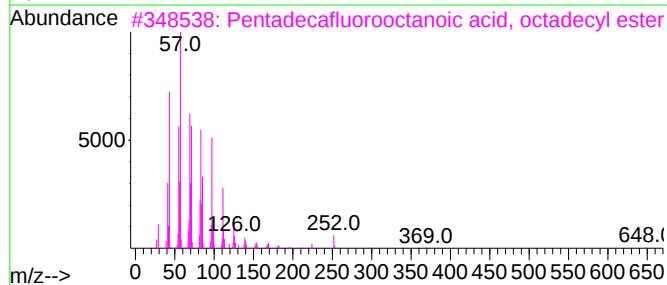
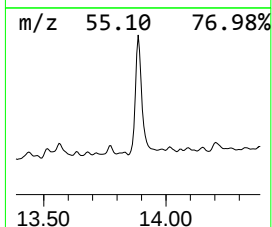
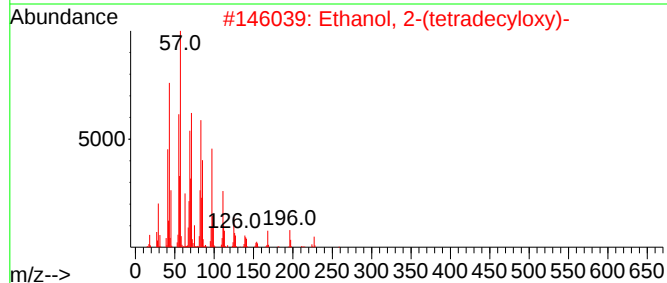
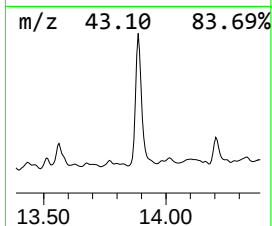
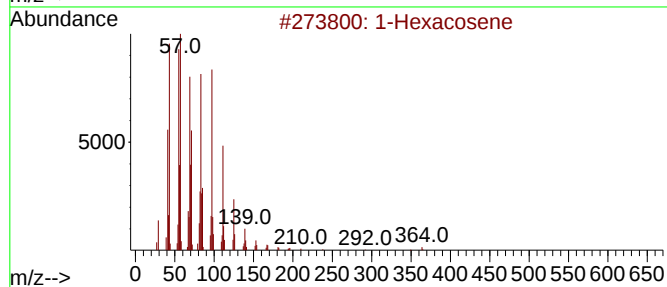
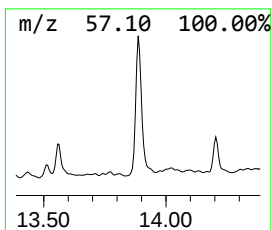
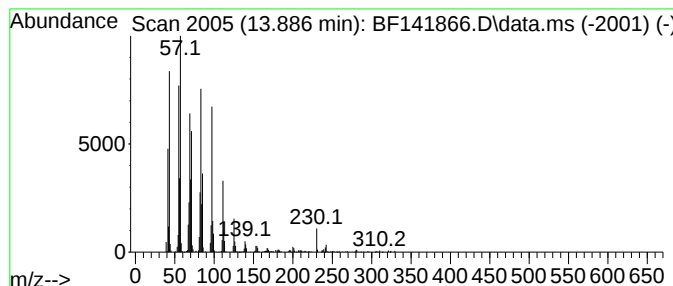
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BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Hexacosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.886	5.04 ng	471751	Chrysene-d12	14.039	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	93
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030625\
Data File : BF141866.D
Acq On : 06 Mar 2025 14:01
Operator : RC/JU
Sample : Q1489-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

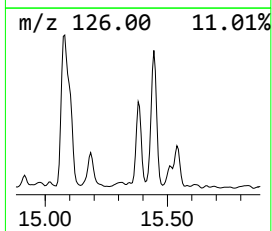
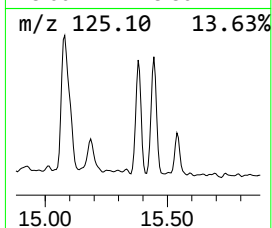
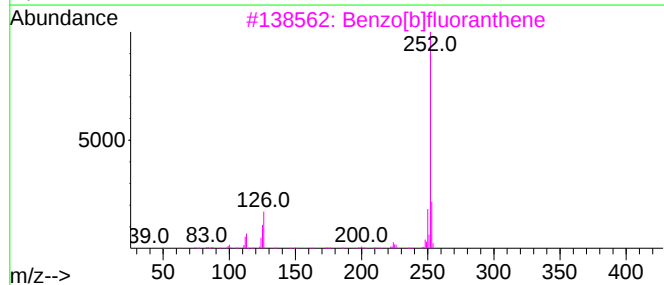
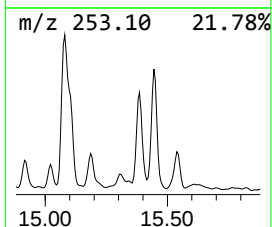
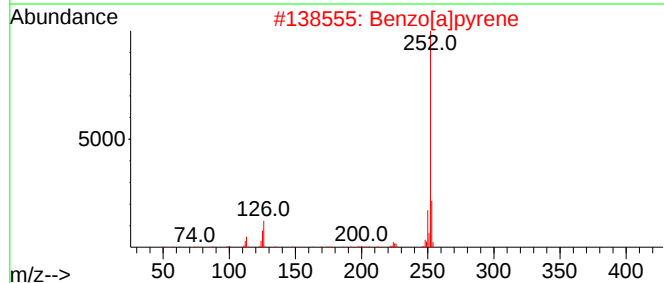
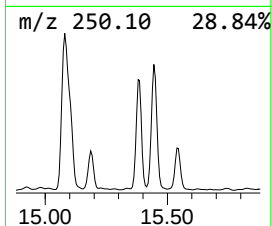
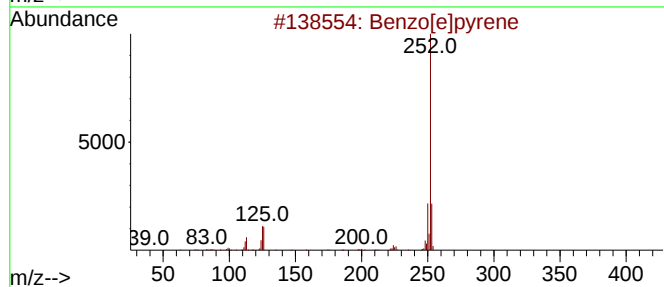
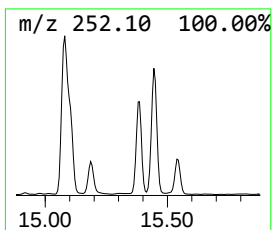
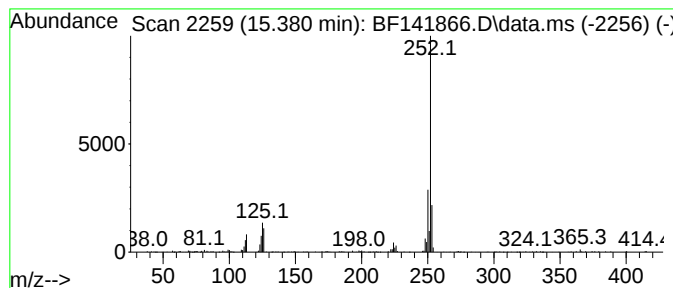
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	3.32 ng	215734	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	98
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5			Perylene	252	C20H12	000198-55-0	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030625\
Data File : BF141866.D
Acq On : 06 Mar 2025 14:01
Operator : RC/JU
Sample : Q1489-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

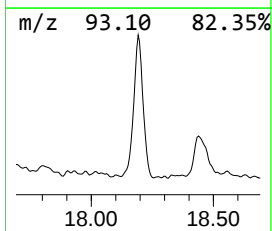
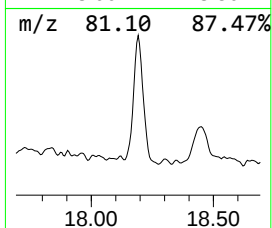
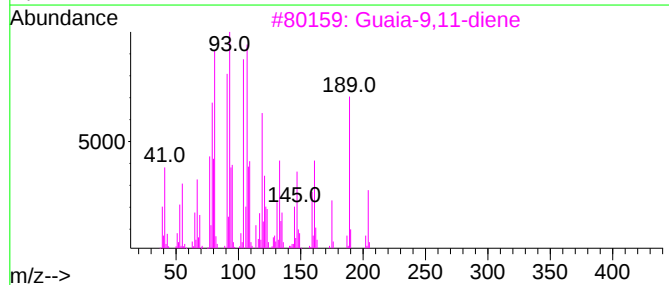
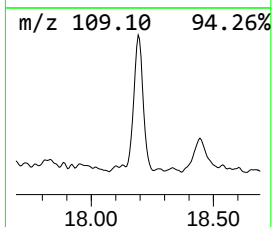
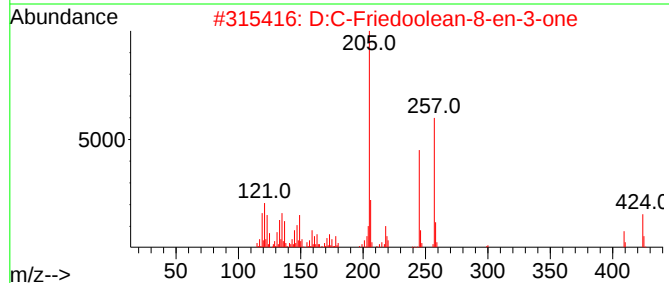
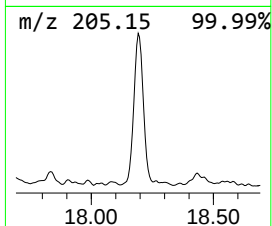
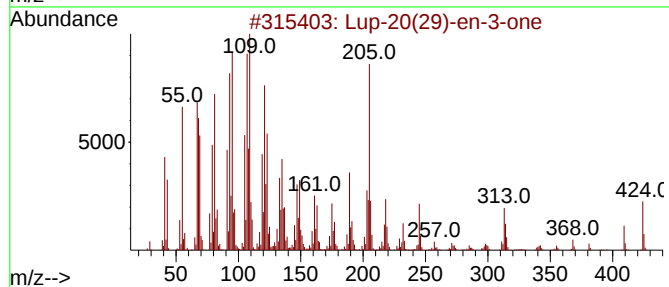
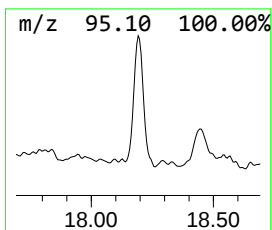
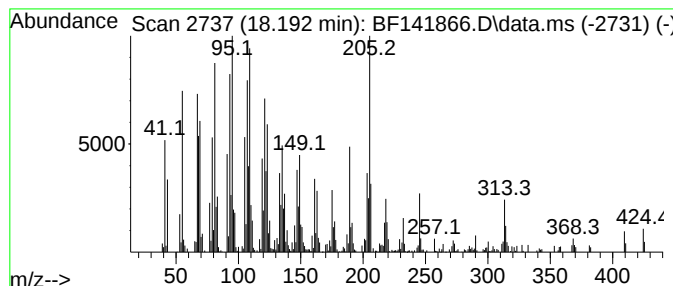
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Lup-20(29)-en-3-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	9.25 ng	601598	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2			D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	86
3			Guaia-9,11-diene	204	C15H24	1000374-19-8	50
4			1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	075023-40-4	45
5			1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030625\
Data File : BF141866.D
Acq On : 06 Mar 2025 14:01
Operator : RC/JU
Sample : Q1489-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022725.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...	2.163	33.7	ng	1601000	1	6.886	949273	20.0
Benzophenone	10.627	5.1	ng	366365	3	9.916	1431480	20.0
n-Hexadecanoic ...	11.927	17.8	ng	1374910	4	11.404	1545210	20.0
4H-Cyclopenta[d...]	12.016	3.4	ng	265871	4	11.404	1545210	20.0
Octadecanoic acid	12.710	7.0	ng	539650	4	11.404	1545210	20.0
1-Hexacosene	13.886	5.0	ng	471751	5	14.039	1870250	20.0
Benzo[e]pyrene	15.380	3.3	ng	215734	6	15.509	1300880	20.0
Lup-20(29)-en-3...	18.192	9.3	ng	601598	6	15.509	1300880	20.0