

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
 Data File : BF143166.D
 Acq On : 18 Jul 2025 14:54
 Operator : RC/JU
 Sample : Q2594-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CC-071325-RW

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-BF071725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.322	14	22	30	rVB	2200445	3574309	33.07%	5.663%
2	4.816	440	446	452	rVB	299975	415962	3.85%	0.659%
3	5.287	519	526	561	rBV	1318073	3347940	30.98%	5.305%
4	5.634	570	585	591	rVB2	3654456	10807966	100.00%	17.125%
5	6.416	713	718	723	rBV	444426	550512	5.09%	0.872%
6	6.575	740	745	754	rVB	459744	571887	5.29%	0.906%
7	6.716	763	769	774	rBV	1899399	2531919	23.43%	4.012%
8	6.928	799	805	807	rBV	810328	1089694	10.08%	1.727%
9	6.957	807	810	814	rVV	751517	1046436	9.68%	1.658%
10	6.998	814	817	824	rVB	105131	128813	1.19%	0.204%
11	7.516	898	905	910	rBV	1899919	2605158	24.10%	4.128%
12	7.881	963	967	973	rBV	88283	118737	1.10%	0.188%
13	8.239	1022	1028	1032	rBV	942965	1243971	11.51%	1.971%
14	8.275	1032	1034	1038	rVV	119378	132967	1.23%	0.211%
15	9.316	1205	1211	1216	rVB	3497450	4530186	41.92%	7.178%
16	9.810	1291	1295	1300	rVB	100377	124939	1.16%	0.198%
17	9.998	1322	1327	1332	rVB	1012826	1256147	11.62%	1.990%
18	10.704	1442	1447	1453	rBV	171786	220074	2.04%	0.349%
19	10.780	1455	1460	1469	rBV	1407944	1815375	16.80%	2.876%
20	11.480	1574	1579	1585	rVB	948169	1183096	10.95%	1.875%
21	11.869	1640	1645	1653	rBV	360206	464623	4.30%	0.736%
22	12.004	1663	1668	1673	rBV	309893	427778	3.96%	0.678%
23	12.063	1675	1678	1684	rVV2	80299	118179	1.09%	0.187%
24	12.786	1797	1801	1810	rBV	168706	256458	2.37%	0.406%
25	13.069	1843	1849	1854	rBV	2490281	3297849	30.51%	5.225%
26	13.651	1926	1948	1953	rBV3	696639	3485554	32.25%	5.523%
27	13.757	1956	1966	1995	rVB2	1134947	5700424	52.74%	9.032%
28	14.116	2022	2027	2034	rVB	535016	709187	6.56%	1.124%
29	15.621	2278	2283	2295	rVB	539788	907932	8.40%	1.439%
30	16.410	2410	2417	2427	rBV3	122058	427294	3.95%	0.677%
31	16.639	2438	2456	2500	rVB	1763955	10022165	92.73%	15.880%

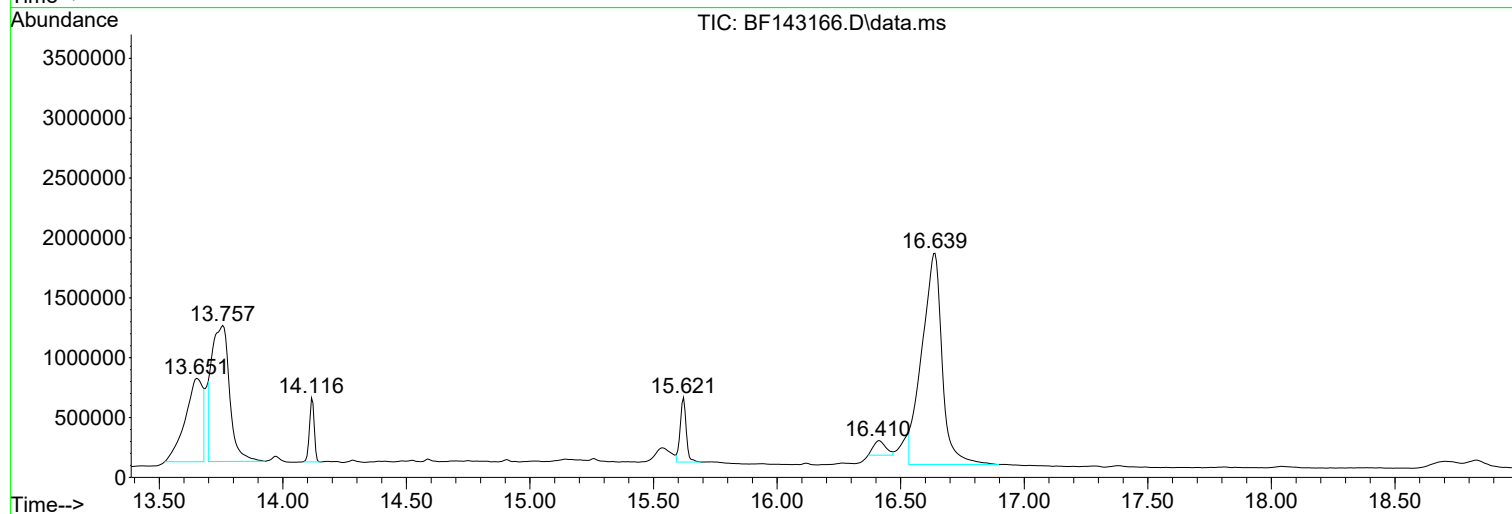
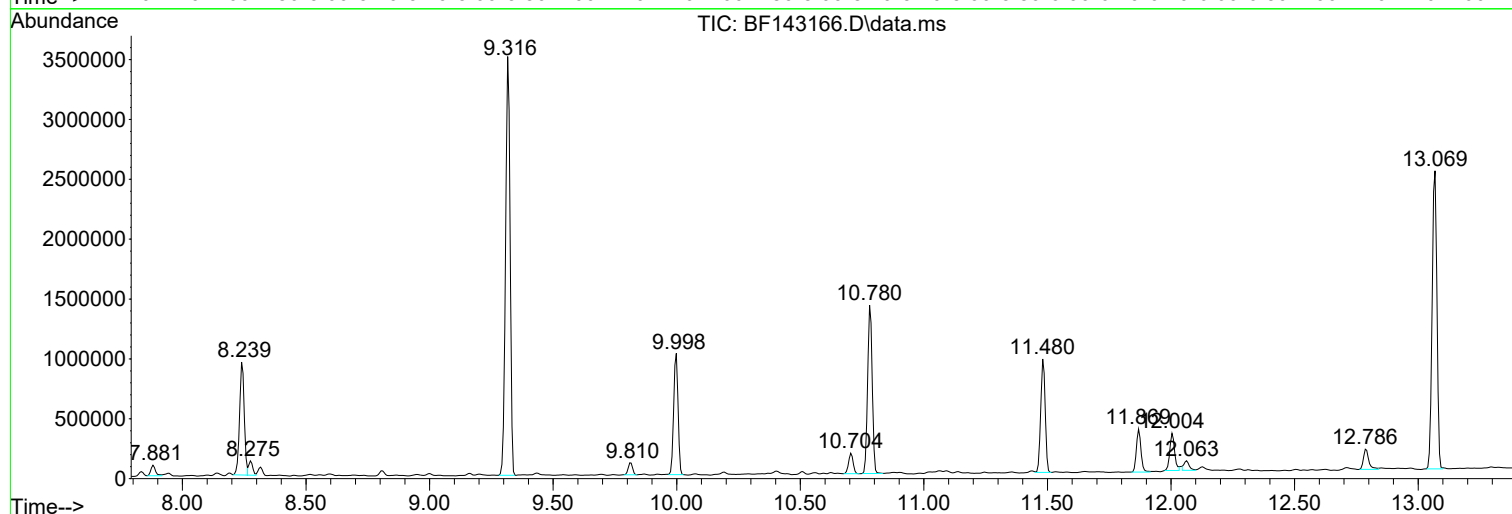
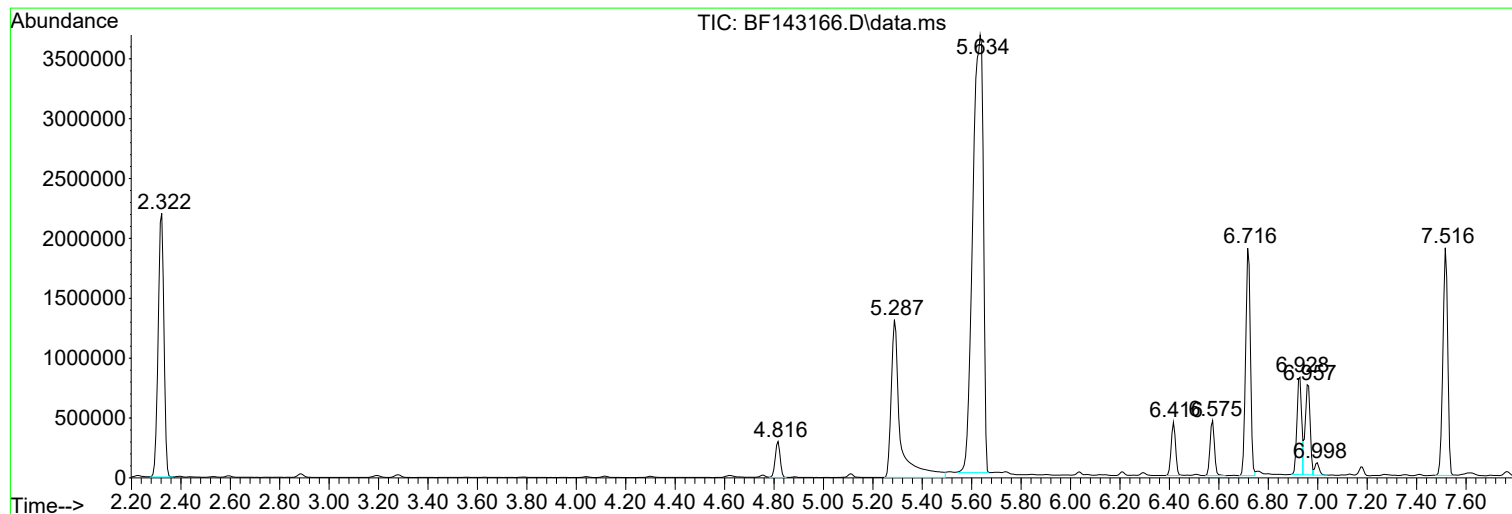
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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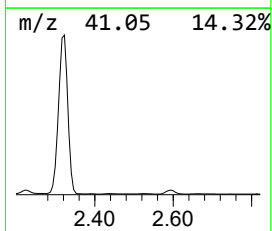
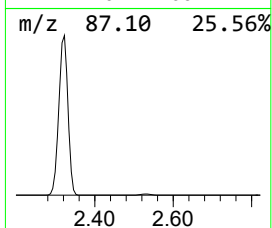
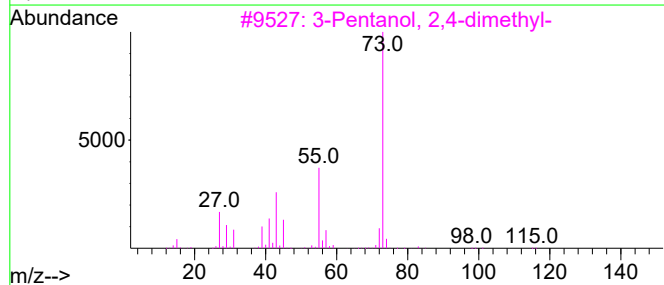
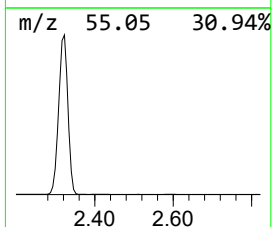
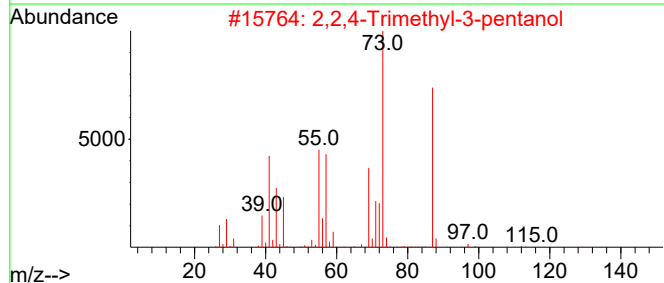
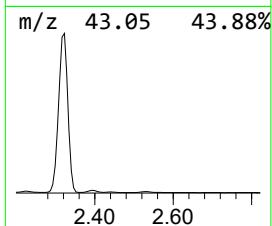
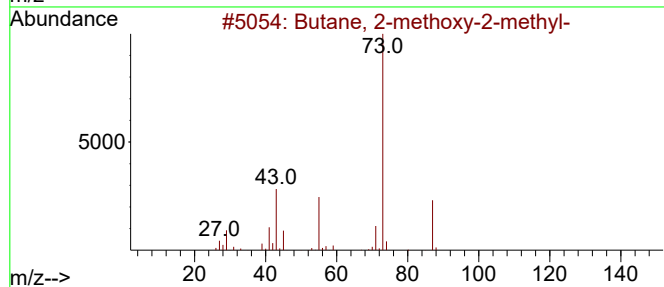
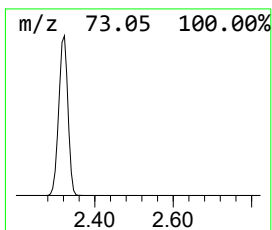
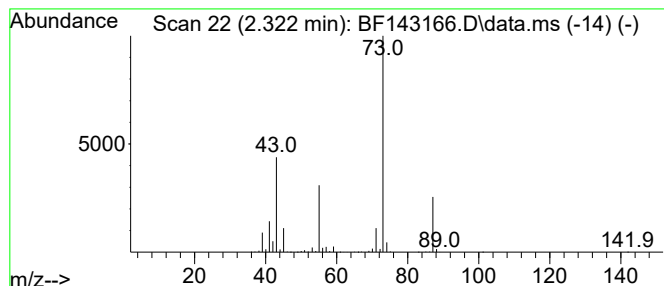
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	68.31 ng	3574310	1,4-Dichlorobenzene-d4	6.963

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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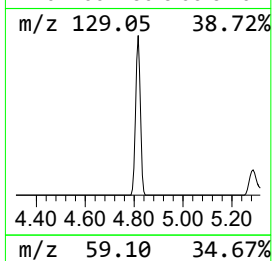
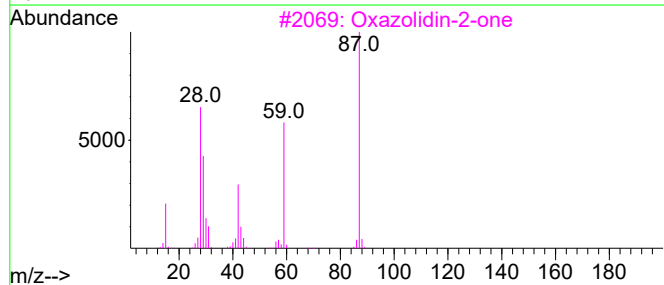
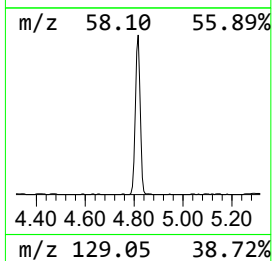
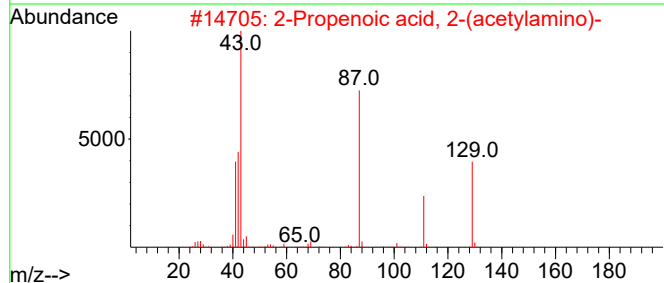
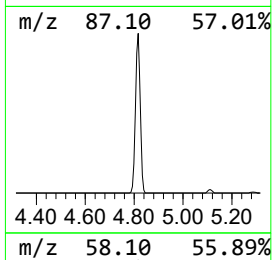
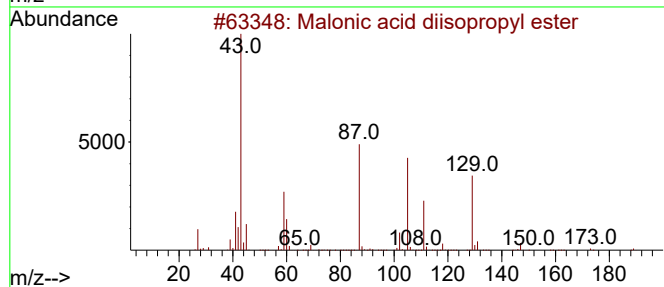
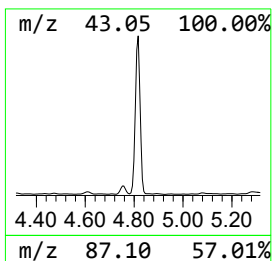
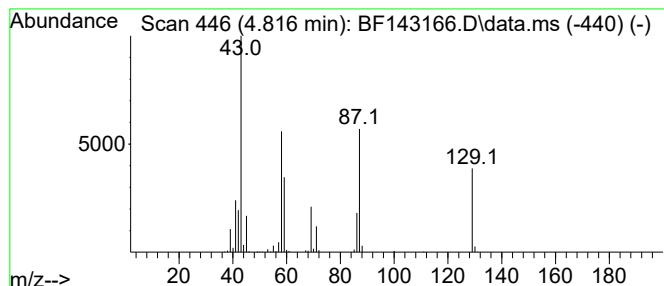
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Malonic acid diisopropyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.816	7.95 ng	415962	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Malonic acid diisopropyl ester	188	C9H16O4	013195-64-7	50
2			2-Propenoic acid, 2-(acetylamino)-	129	C5H7NO3	005429-56-1	32
3			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	30
4			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	30
5			Oxirane, 2,3-diethyl-	100	C6H12O	004468-66-0	22



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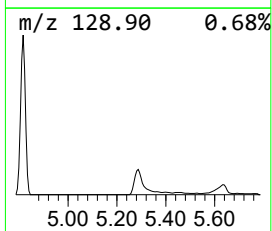
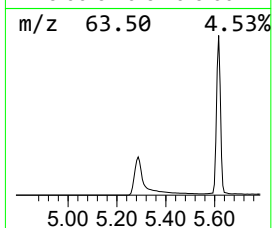
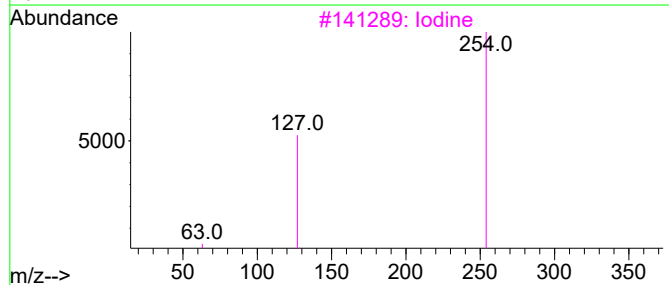
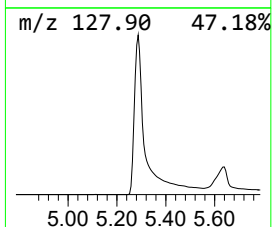
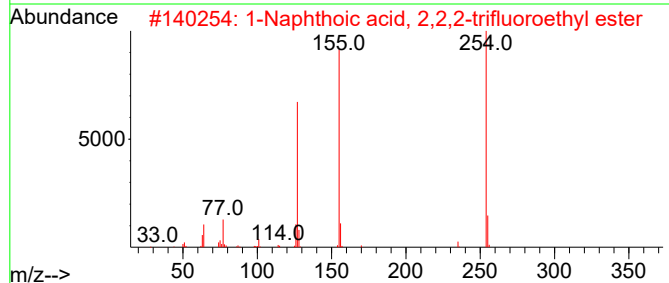
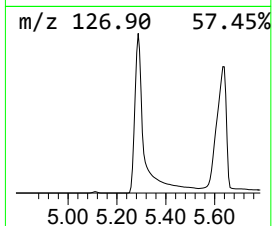
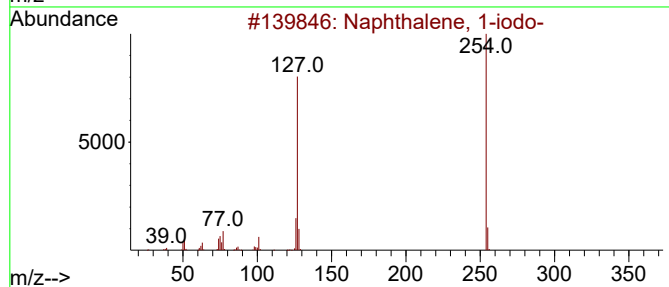
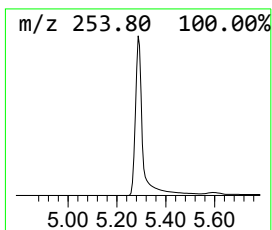
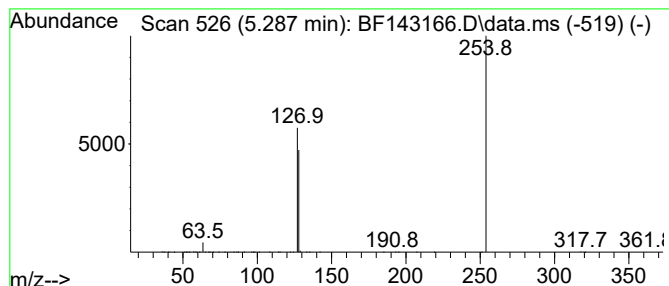
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown5.287 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.287	63.99 ng	3347940	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-iodo-	254	C10H7I	000090-14-2	9
2			1-Naphthoic acid, 2,2,2-trifluor...	254	C13H9F3O2	1000325-54-4	9
3			Iodine	254	I2	007553-56-2	9
4			5-Chloro-3-iodo-2-pyridinylamine	254	C5H4ClIN2	211308-81-5	7
5			Acenaphtho(1,2-b)quinoxaline	254	C18H10N2	000207-11-4	5



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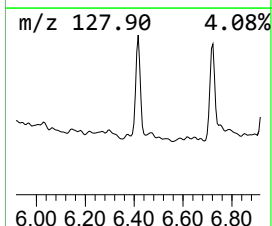
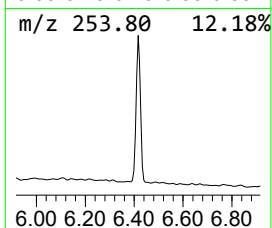
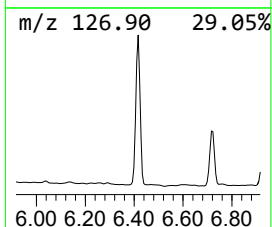
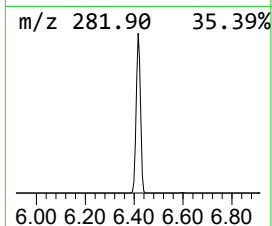
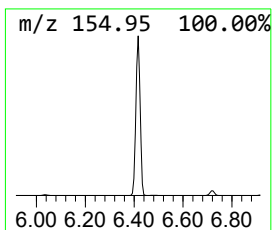
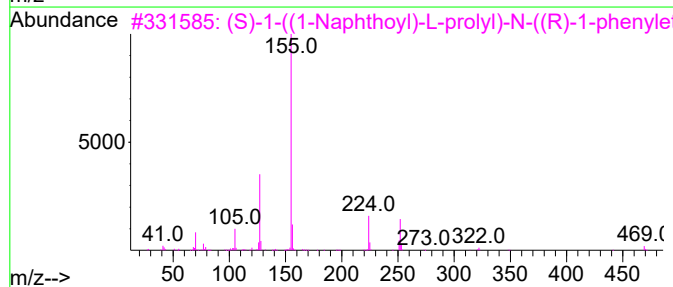
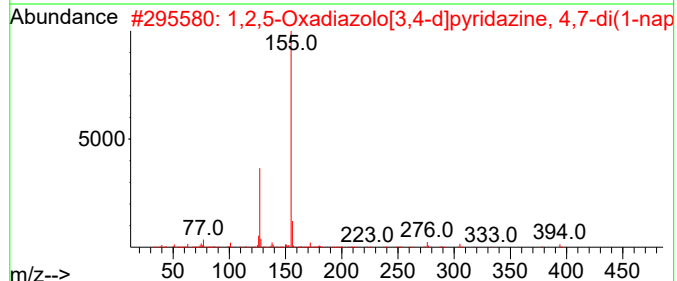
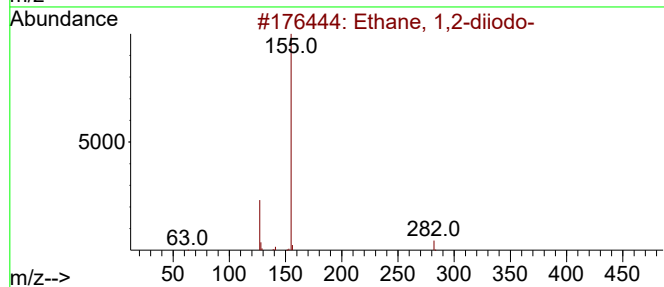
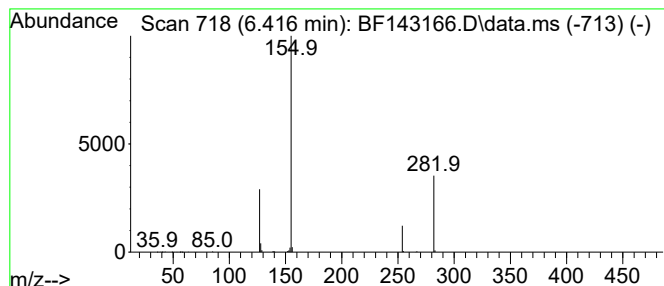
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethane, 1,2-diiodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.416	10.52 ng	550512	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-diiodo-	282	C2H4I2	000624-73-7	72
2			1,2,5-Oxadiazolo[3,4-d]pyridazin...	390	C24H14N4O2	1000276-89-8	9
3			(S)-1-((1-Naphthoyl)-L-prolyl)-N...	469	C29H31N3O3	1000483-34-9	9
4			2-Chloro-4-fluorobenzonitrile	155	C7H3ClFN	060702-69-4	7
5			2-Chloro-6-fluorobenzonitrile	155	C7H3ClFN	000668-45-1	7



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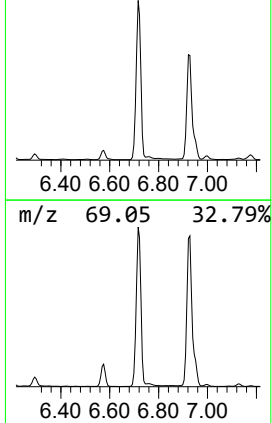
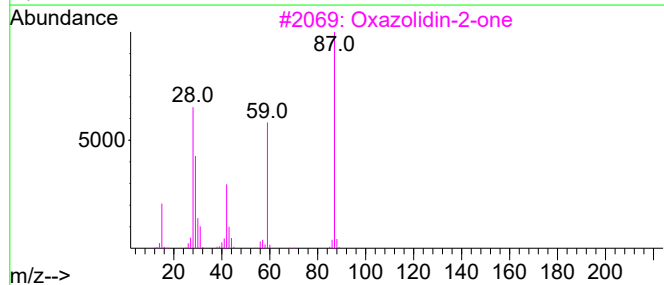
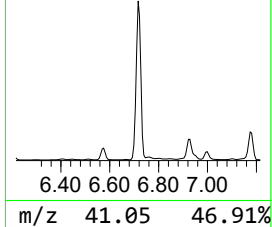
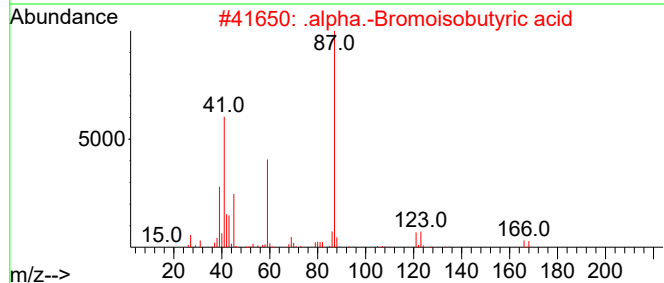
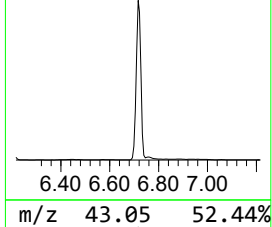
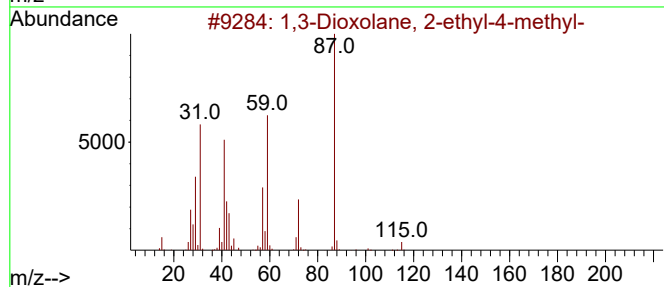
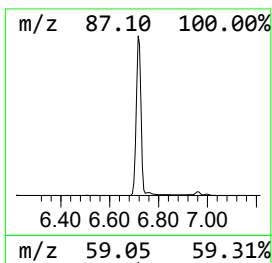
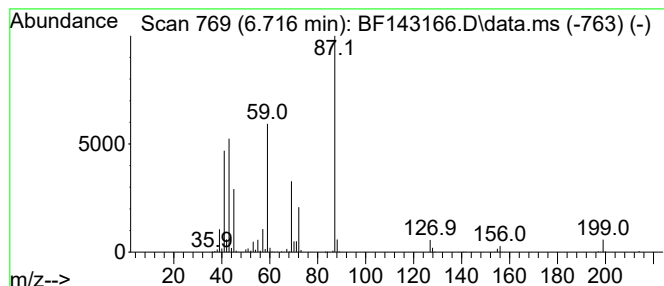
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.716	48.39 ng	2531920	1,4-Dichlorobenzene-d4	6.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	59
2		.alpha.-Bromoisobutyric acid	166	C4H7BrO2	002052-01-9	59
3		Oxazolidin-2-one	87	C3H5NO2	000497-25-6	52
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	49
5		N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	47



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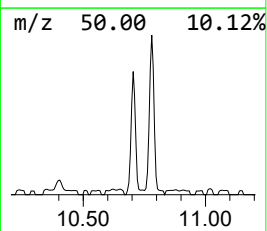
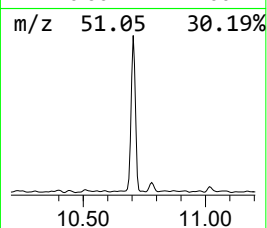
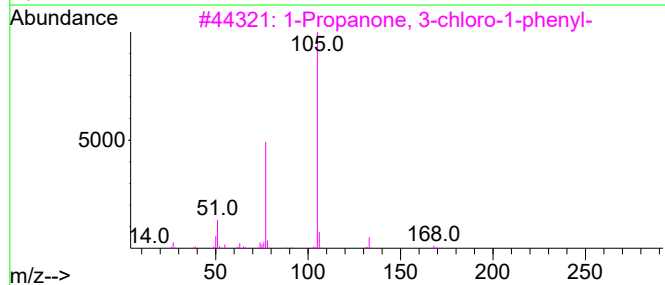
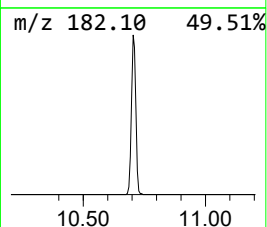
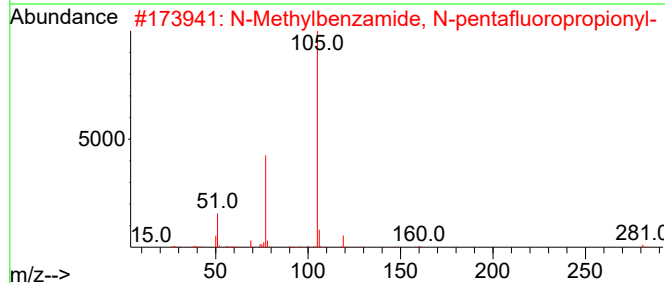
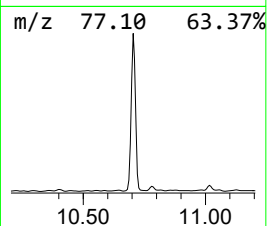
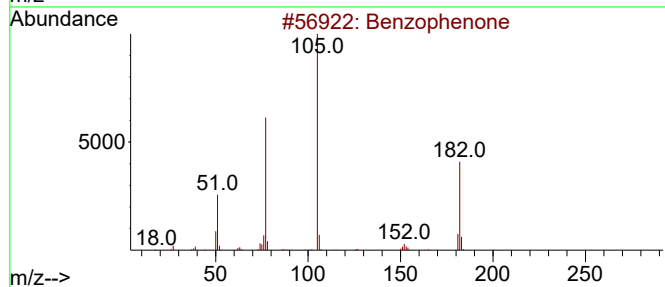
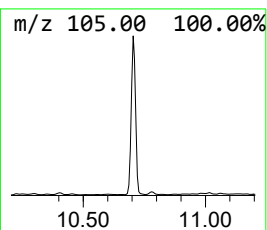
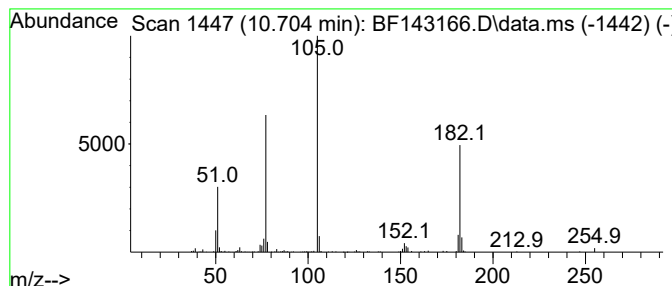
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.704	3.50 ng	220074	Acenaphthene-d10	9.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50
4			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	50
5			Benzoylformic acid	150	C8H6O3	000611-73-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
Sample : Q2594-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

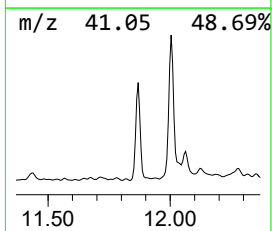
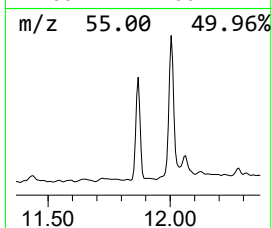
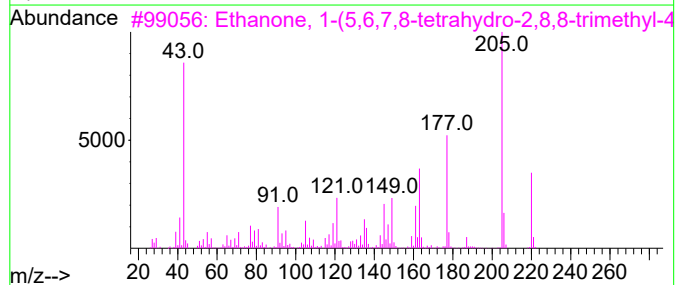
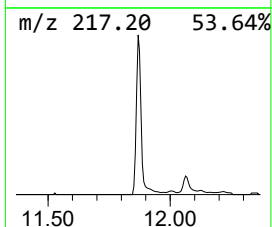
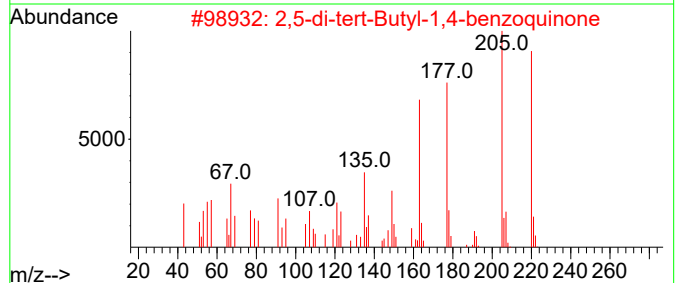
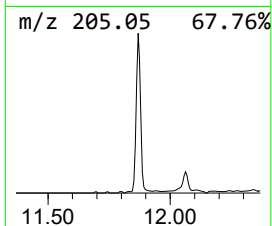
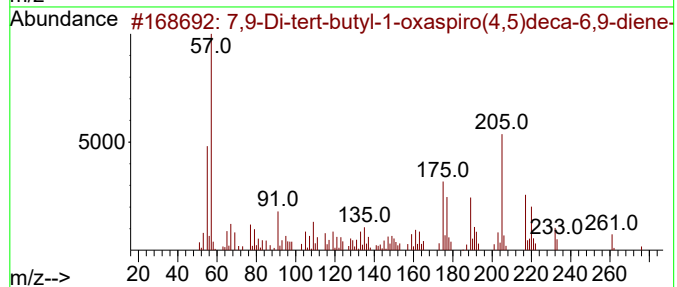
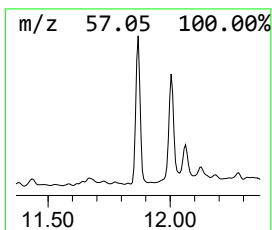
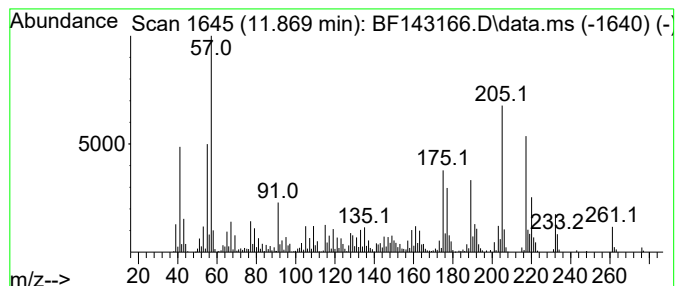
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.869	7.85 ng	464623	Phenanthrene-d10		11.480	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...		276	C17H24O3	082304-66-3	99
2	2,5-di-tert-Butyl-1,4-benzoquinone		220	C14H20O2	002460-77-7	60
3	Ethanone, 1-(5,6,7,8-tetrahydro-...		220	C14H20O2	071596-88-8	46
4	2-Phenazinecarbonitrile		205	C13H7N3	006479-93-2	40
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...		220	C15H24O	104188-25-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
Sample : Q2594-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CC-071325-RW

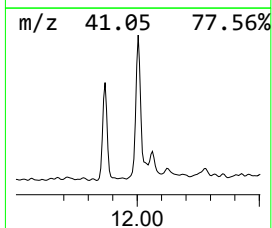
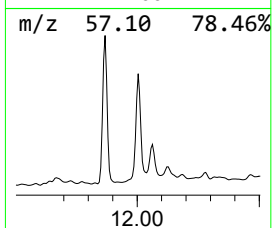
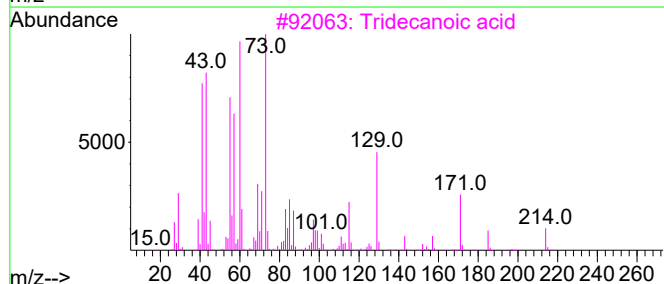
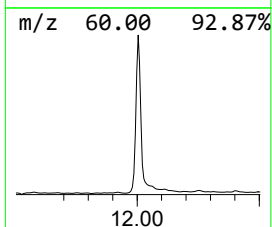
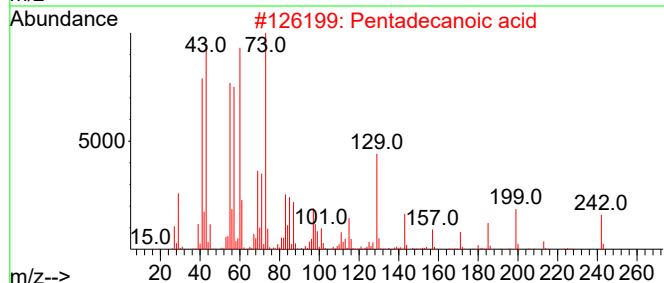
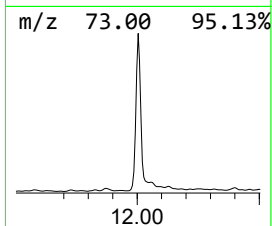
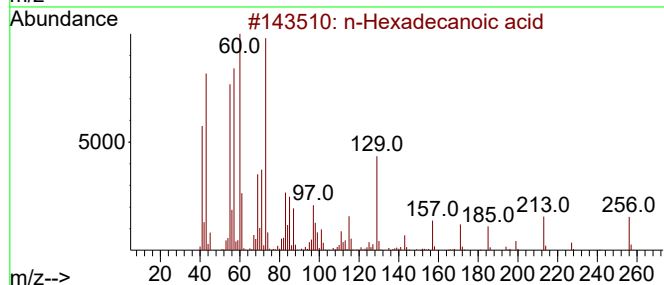
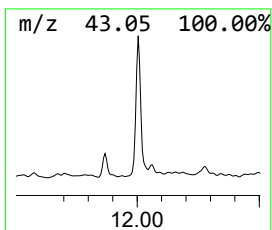
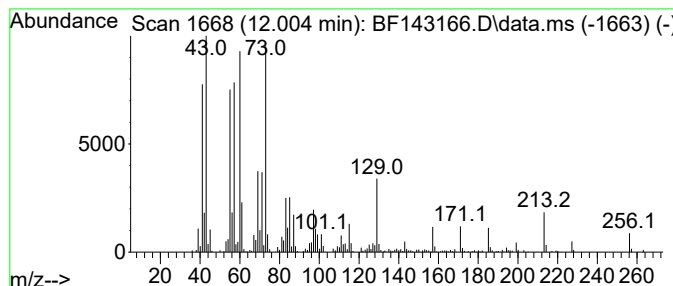
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	7.23 ng	427778	Phenanthrene-d10	11.480

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
Sample : Q2594-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CC-071325-RW

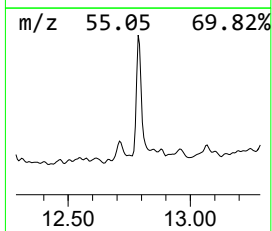
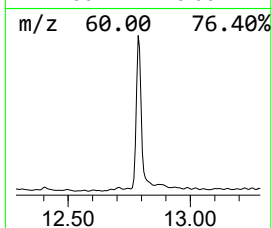
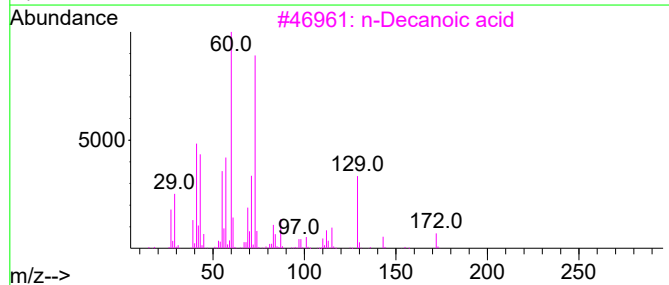
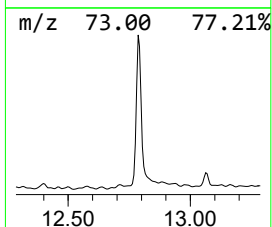
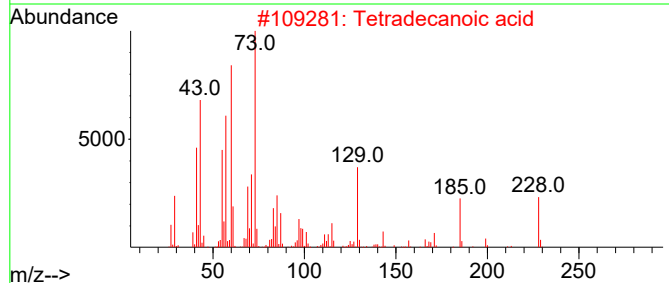
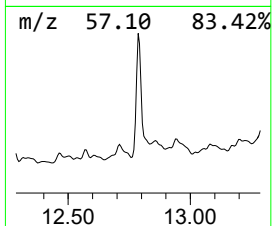
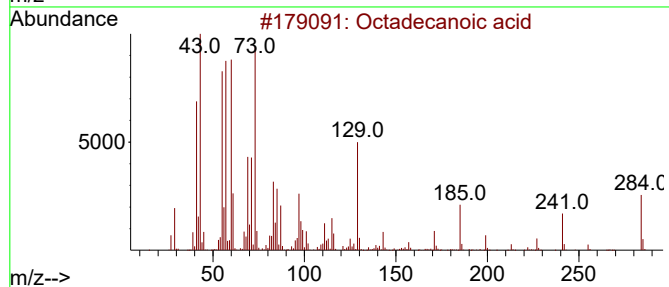
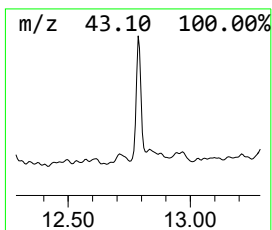
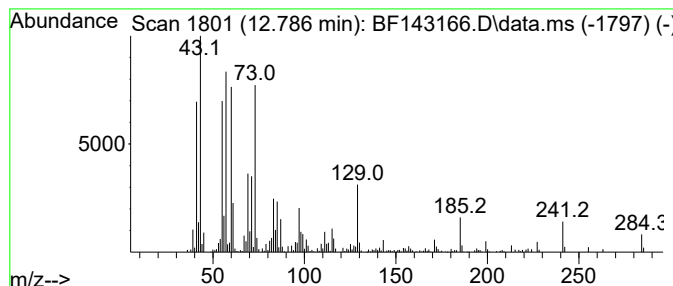
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	4.34 ng	256458	Phenanthrene-d10	11.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	60
4			Nonanoic acid	158	C9H18O2	000112-05-0	46
5			Octanoic acid	144	C8H16O2	000124-07-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
Sample : Q2594-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

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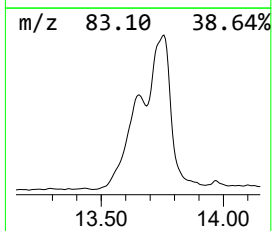
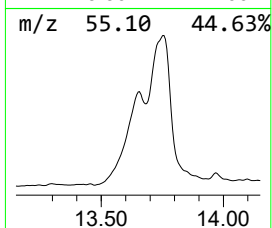
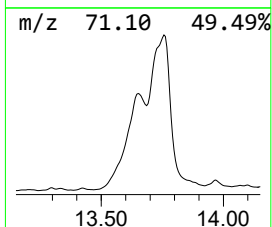
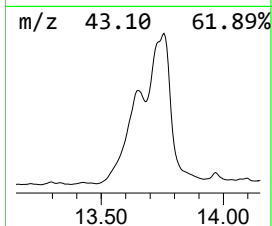
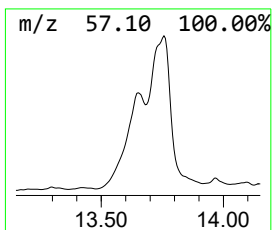
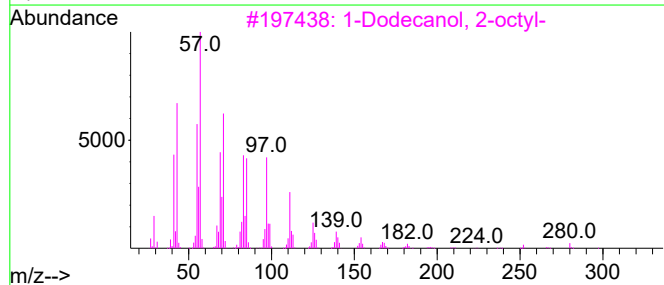
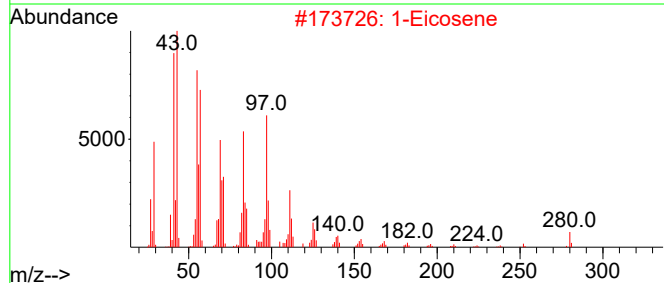
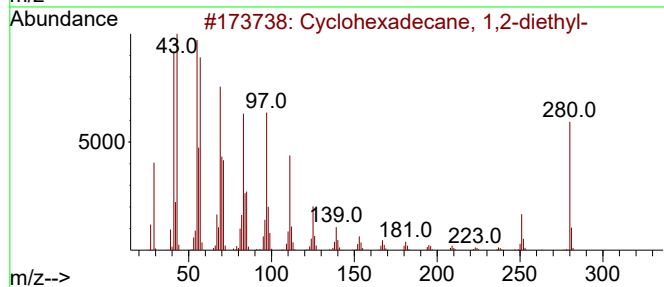
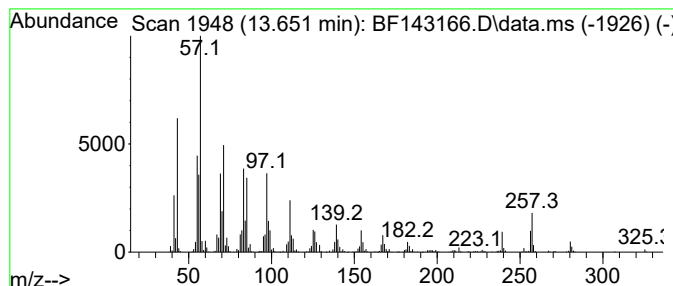
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexadecane, 1,2-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.651	98.30 ng	3485550	Chrysene-d12	14.116

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
2		1-Eicosene	280	C20H40	003452-07-1	87
3		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
4		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	76
5		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
Sample : Q2594-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CC-071325-RW

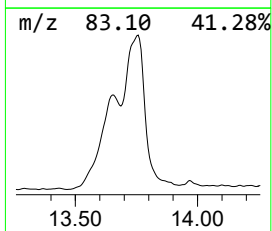
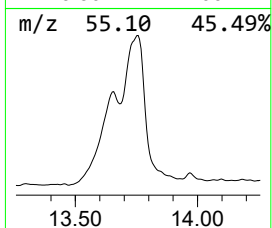
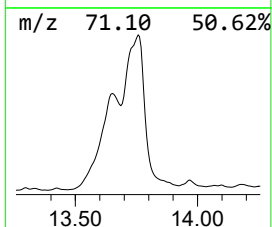
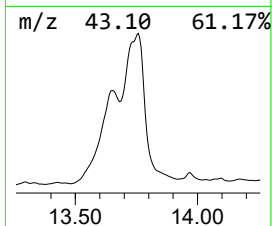
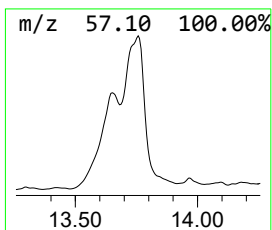
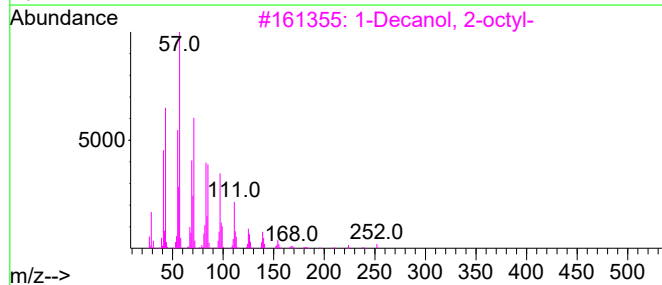
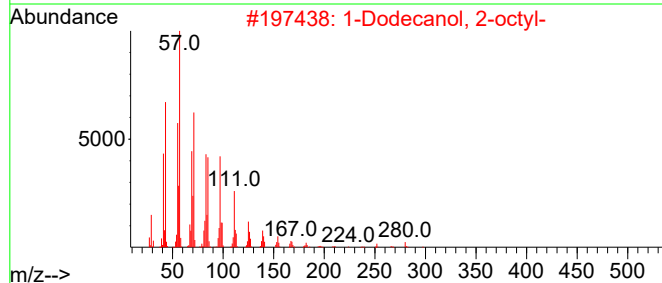
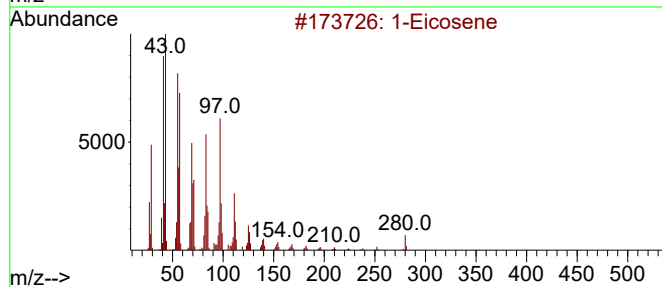
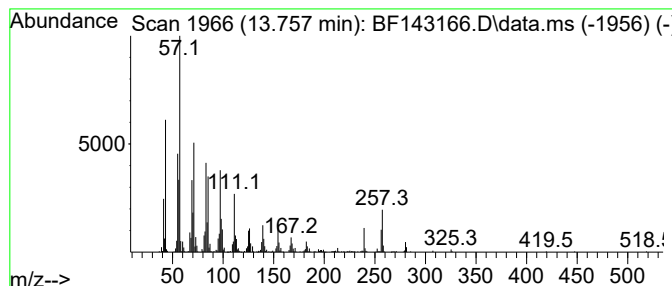
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Eicosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	160.76 ng	5700420	Chrysene-d12	14.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Eicosene	280	C20H40	003452-07-1	87
2			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	76
3			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	70
4			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	68
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
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ALS Vial : 9 Sample Multiplier: 1

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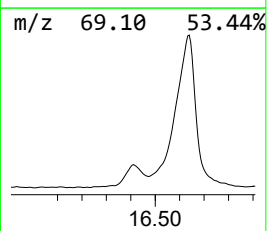
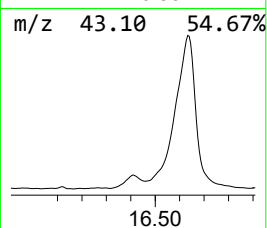
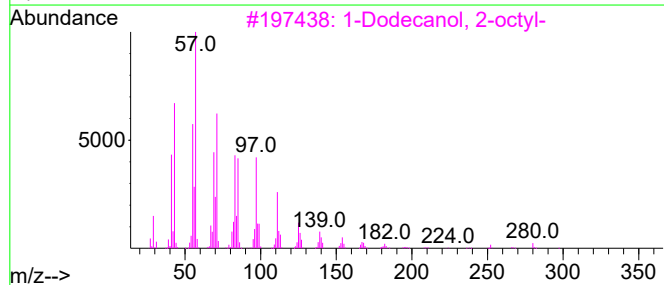
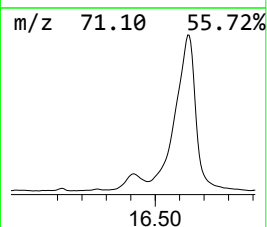
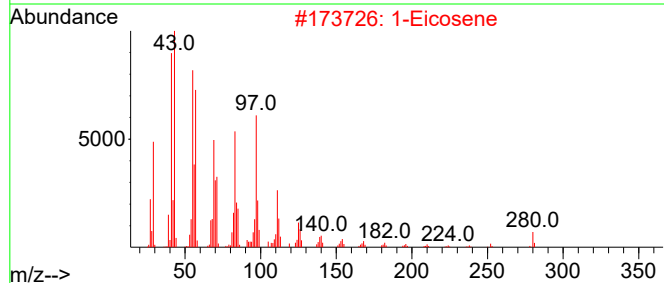
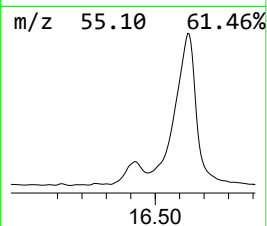
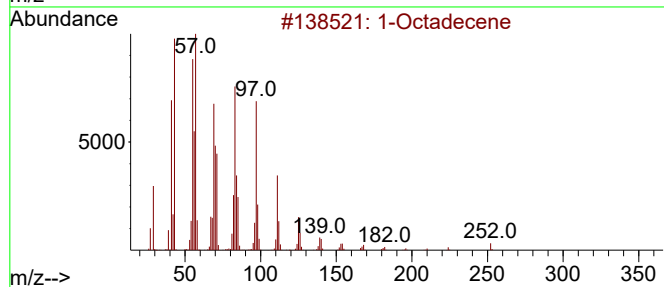
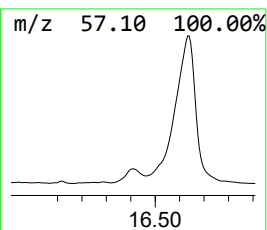
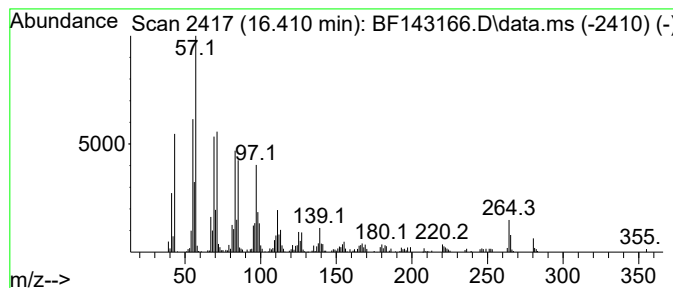
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Octadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.410	9.41 ng	427294	Perylene-d12	15.621

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecene	252	C18H36	000112-88-9	86
2		1-Eicosene	280	C20H40	003452-07-1	83
3		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	68
5		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
Sample : Q2594-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CC-071325-RW

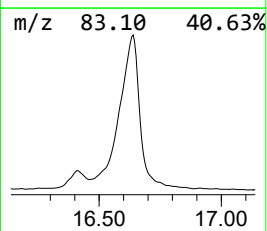
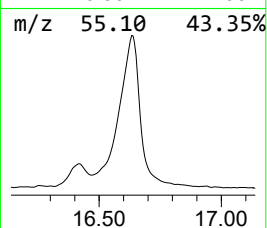
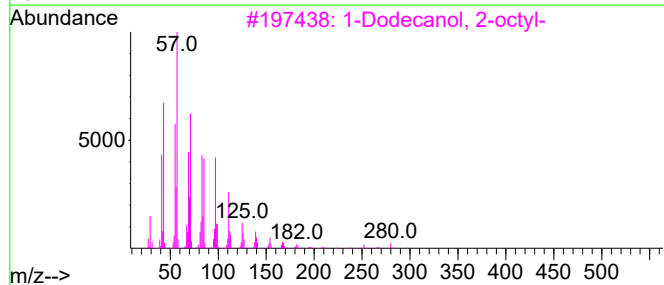
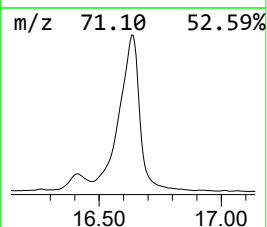
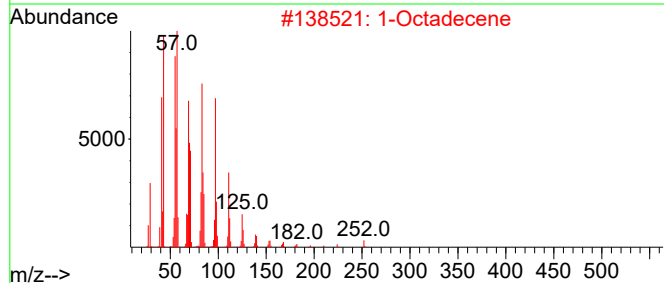
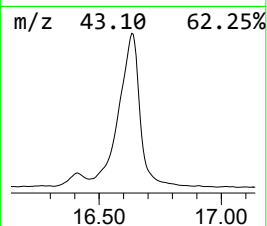
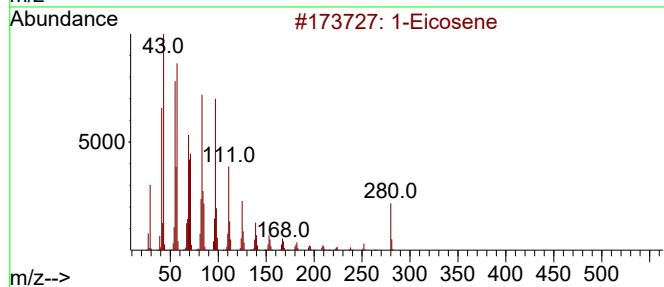
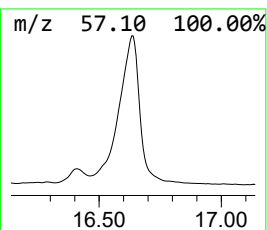
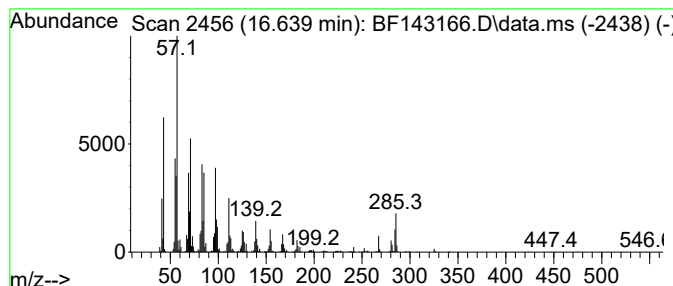
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Dodecanol, 2-octyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.639	220.77 ng	10022200	Perylene-d12	15.621

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Eicosene	280	C20H40	003452-07-1	90
2		1-Octadecene	252	C18H36	000112-88-9	87
3		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
4		2-Octyldodecyl isobutyrate	368	C24H48O2	1000368-55-5	87
5		Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071825\
Data File : BF143166.D
Acq On : 18 Jul 2025 14:54
Operator : RC/JU
Sample : Q2594-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CC-071325-RW

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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...	2.322	68.3	ng	3574310	1	6.963	1046440	20.0
Malonic acid di...	4.816	8.0	ng	415962	1	6.963	1046440	20.0
unknown5.287	5.287	64.0	ng	3347940	1	6.963	1046440	20.0
Ethane, 1,2-dii...	6.416	10.5	ng	550512	1	6.963	1046440	20.0
1,3-Dioxolane, ...	6.716	48.4	ng	2531920	1	6.963	1046440	20.0
Benzophenone	10.704	3.5	ng	220074	3	9.998	1256150	20.0
7,9-Di-tert-but...	11.869	7.8	ng	464623	4	11.480	1183100	20.0
n-Hexadecanoic ...	12.004	7.2	ng	427778	4	11.480	1183100	20.0
Octadecanoic acid	12.786	4.3	ng	256458	4	11.480	1183100	20.0
Cyclohexadecane...	13.651	98.3	ng	3485550	5	14.116	709187	20.0
1-Eicosene	13.757	160.8	ng	5700420	5	14.116	709187	20.0
1-Octadecene	16.410	9.4	ng	427294	6	15.621	907932	20.0
1-Dodecanol, 2-...	16.639	220.8	ng	10022200	6	15.621	907932	20.0