LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
Data File : BF130041.D
Acq On : 29 Aug 2022 18:49
Operator : CG\JU
Sample : N4355-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-34

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: BF130041.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.875	91	100	106	rBV	90457	165421	3.69%	0.681%
2	4.157	309	318	324	rBV2	90277	144800	3.23%	0.596%
3	4.252	329	334	339	rVB2	117892	177195	3.96%	0.729%
4	4.910	443	446	456	rBV	223801	318198	7.11%	1.309%
5	5.340	516	519	533	rBV	1663560	1882230	42.04%	7.746%
6	5.716	580	583	587	rBV	67551	69120	1.54%	0.284%
7	6.369	691	694	709	rBV	1119672	1273634	28.45%	5.241%
8	6.698	747	750	756	rBV	746360	683383	15.26%	2.812%
9	6.769	759	762	767	rBV	56379	53767	1.20%	0.221%
10	6.940	785	791	794	rBV3	55785	122395	2.73%	0.504%
11	6.998	795	801	806	rVV	150494	289471	6.47%	1.191%
12	7.045	806	809	813	rVB2	57416	63997	1.43%	0.263%
13	7.275	844	848	851	rBV	2609856	2599795	58.07%	10.699%
14	7.310	851	854	858	rVV3	314951	639985	14.29%	2.634%
15	7.351	858	861	866	rVB2	375859	551934	12.33%	2.271%
16	7.563	890	897	900	rBV2	179737	220976	4.94%	0.909%
17	7.928	952	959	965	rVB4	41958	71568	1.60%	0.295%
18	7.981	965	968	978	rBV	1062622	956760	21.37%	3.937%
19	8.216	1002	1008	1011	rBV5	27563	54264	1.21%	0.223%
20	8.281	1015	1019	1025	rVV3	73145	146728	3.28%	0.604%
21	8.534	1057	1062	1067	rBV3	37181	85447	1.91%	0.352%
22	8.592	1070	1072	1079	rVB2	57300	66032	1.47%	0.272%
23	8.734	1093	1096	1105	rVB4	46020	85379	1.91%	0.351%
24	8.804	1105	1108	1113	rBV2	65785	76341	1.71%	0.314%
25	8.881	1114	1121	1126	rBV8	37656	96739	2.16%	0.398%
26	9.057	1146	1151	1154	rBV	5070614	4477179	100.00%	18.425%
27	9.734	1262	1266	1270	rBV	1261530	1037839	23.18%	4.271%
28	10.533	1398	1402	1405	rBV	3107828	2682271	59.91%	11.038%
29	11.222	1516	1519	1524	rVB	1039099	931717	20.81%	3.834%
30	11.751	1606	1609	1620	rVB2	98284	132338	2.96%	0.545%
31	12.804	1784	1788	1792	rBV	3134198	2838109	63.39%	11.680%
32	13.745	1944	1948	1959	rVB5	38354	76140	1.70%	0.313%
33	13.869	1966	1969	1974	rBV	636610	548999	12.26%	2.259%
34	15.298	2208	2212	2222	rVB	550542	679489	15.18%	2.796%

Sum of corrected areas: 24299640

Instrument :
BNA_F
ClientSampleId :
MW-34

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
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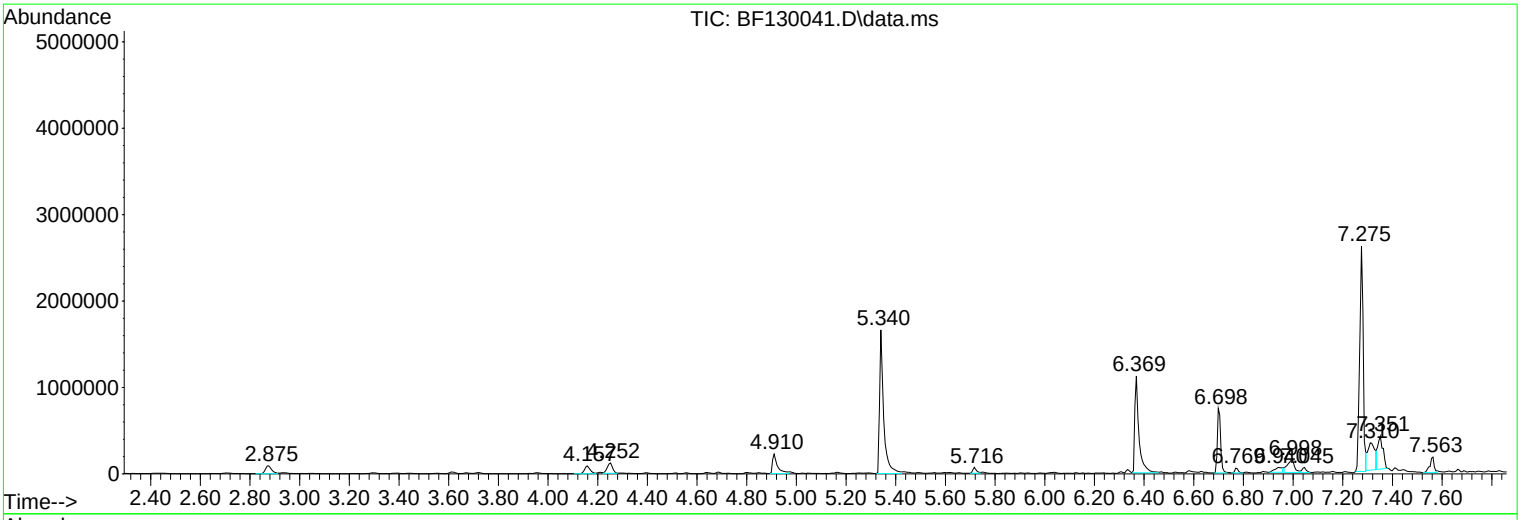
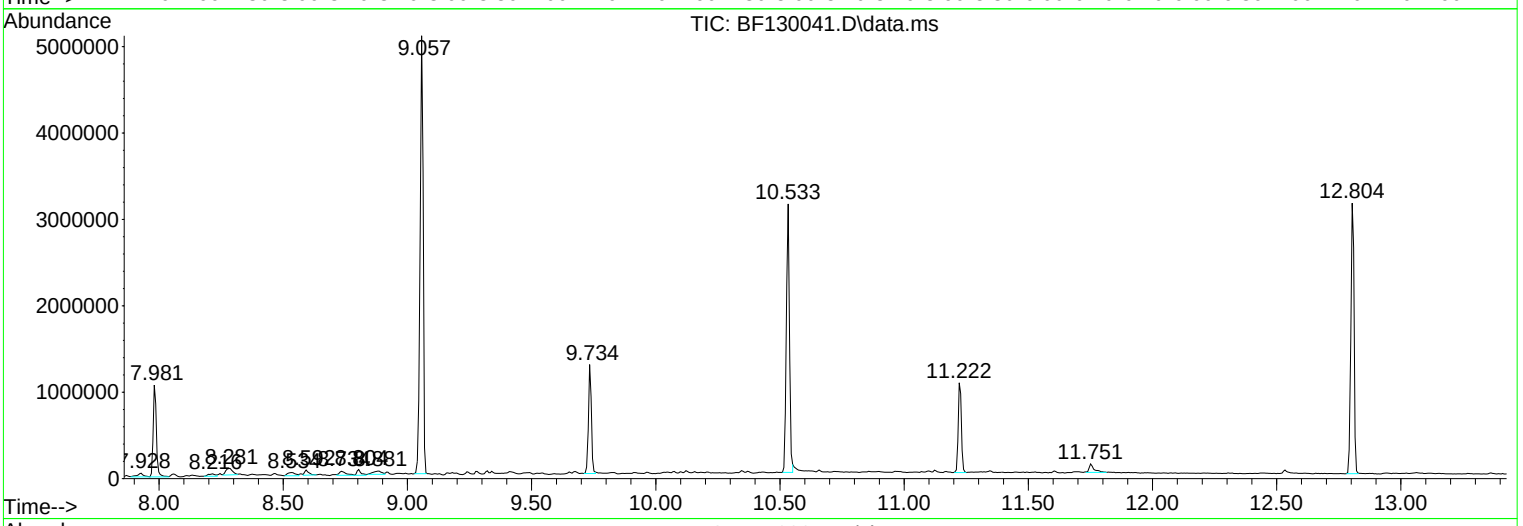
Operator : CG\JU
Sample : N4355-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

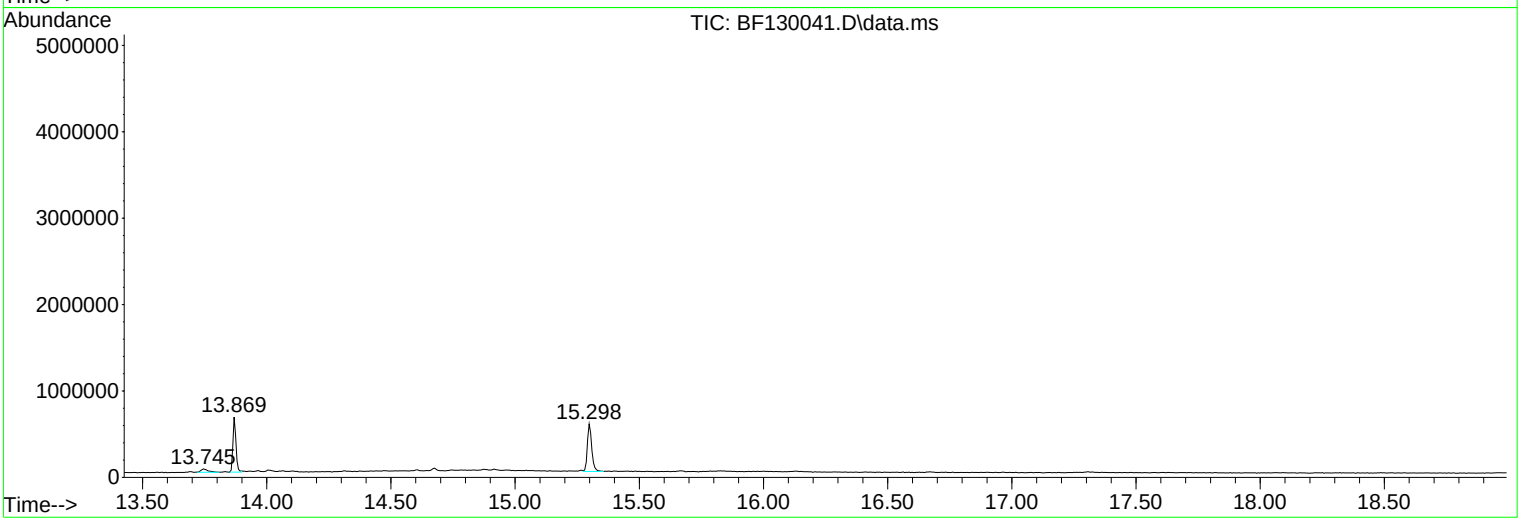
Instrument :
BNA_F
ClientSampleId :
MW-34

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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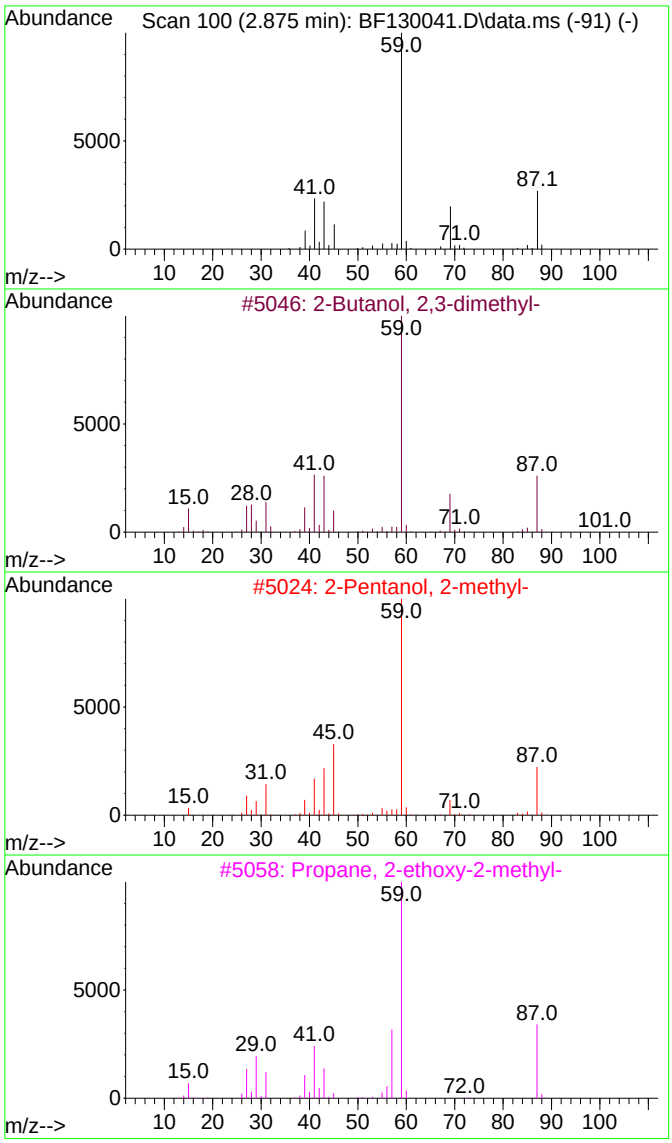
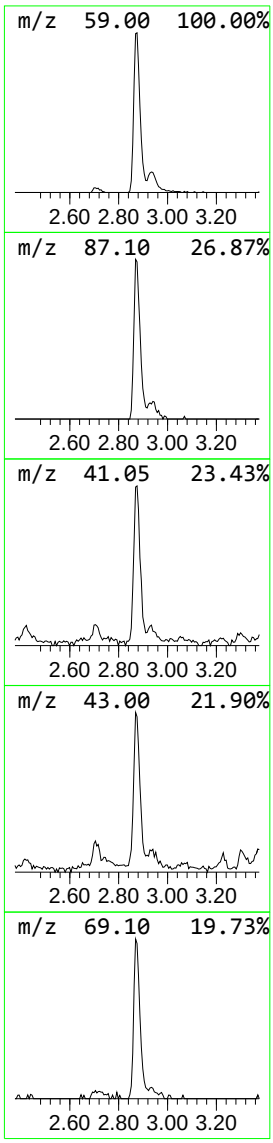
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.875	4.84 ng	165421	1,4-Dichlorobenzene-d4	6.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
4	Propane, 1-ethoxy-	88	C5H12O	000628-32-0	53
5	Amylene hydrate	88	C5H12O	000075-85-4	42





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Operator : CG\JU
Sample : N4355-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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
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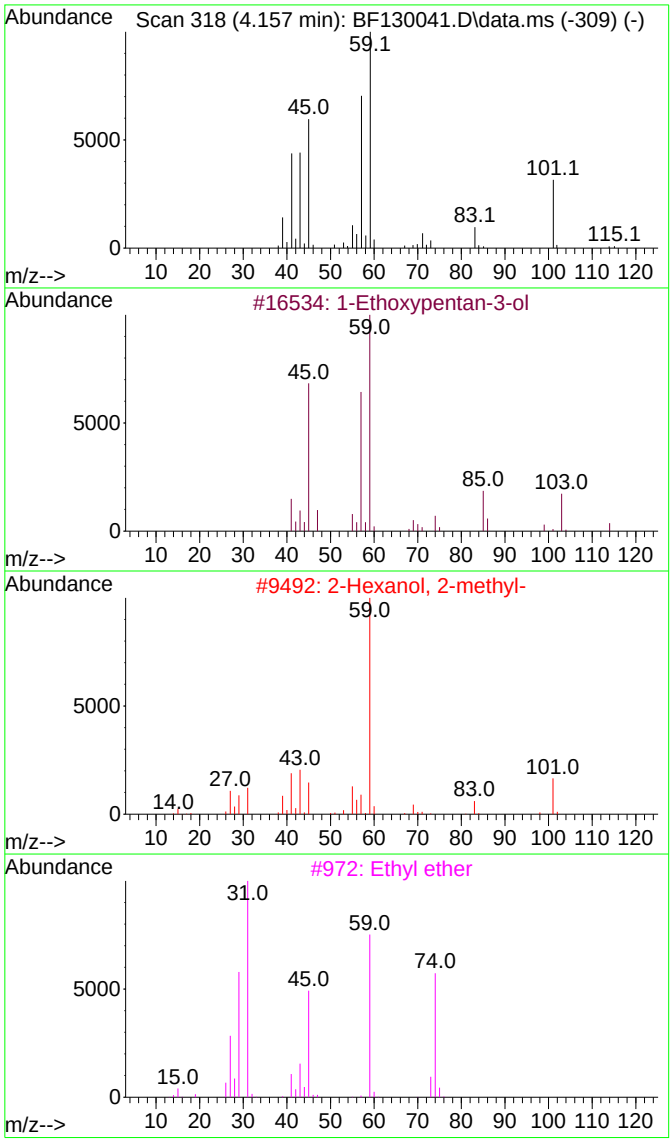
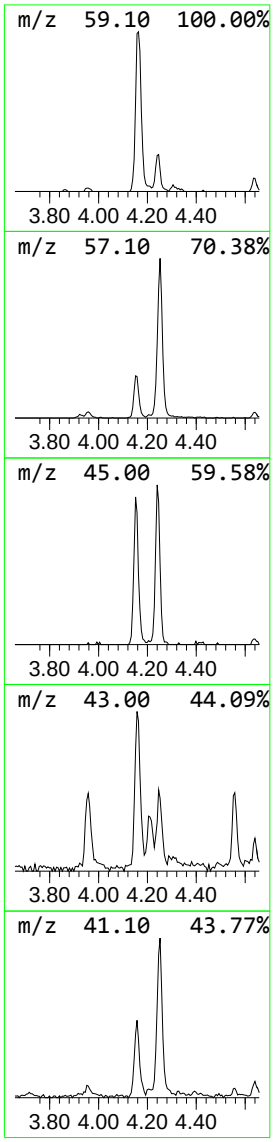
****

Peak Number 2 1-Ethoxypentan-3-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.157	4.24 ng	144800	1,4-Dichlorobenzene-d4	6.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethoxypentan-3-ol	132	C7H16O2	100910-92-7	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	45
3	Ethyl ether	74	C4H10O	000060-29-7	45
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	43
5	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	42





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Operator : CG\JU
Sample : N4355-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

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

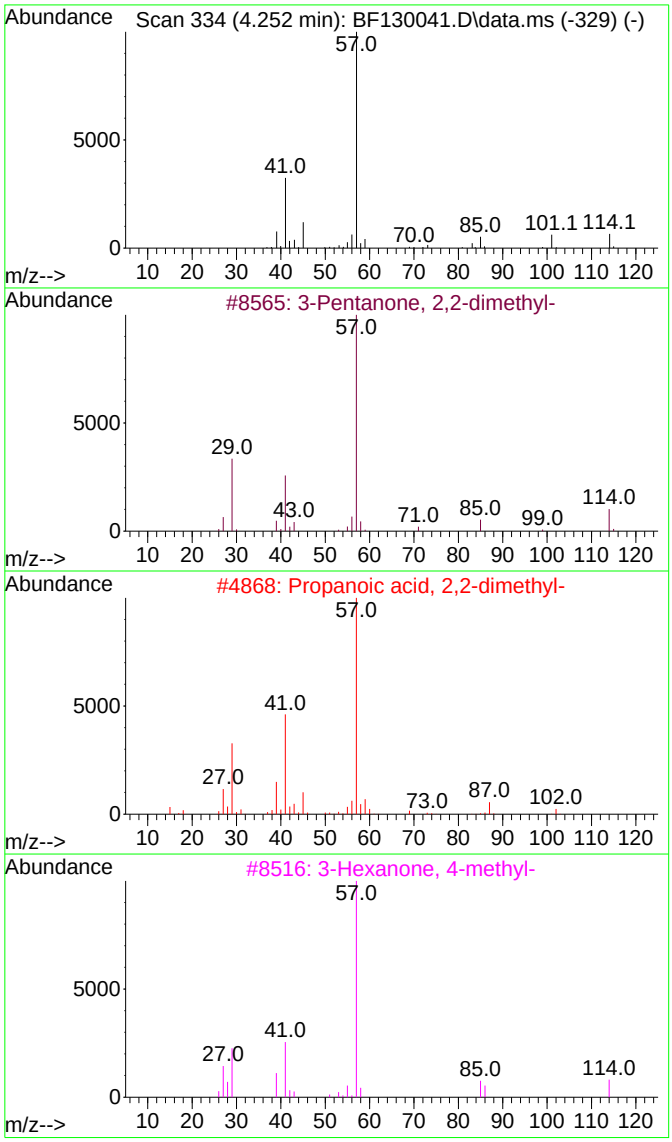
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

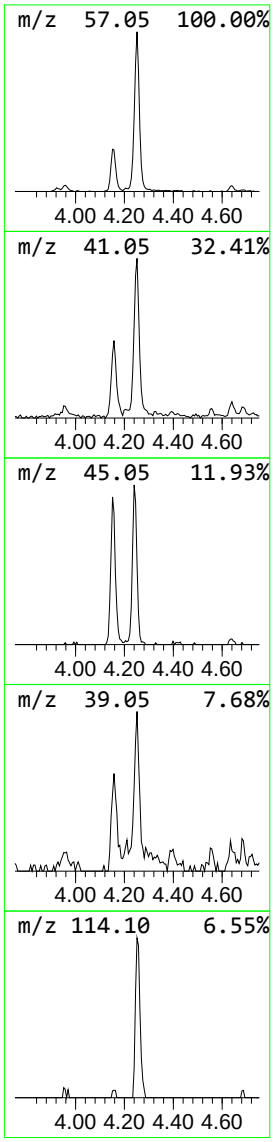
****

Peak Number 3 unknown4.252 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.252	5.19 ng	177195	1,4-Dichlorobenzene-d4	6.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	49
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	25
3	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	17
4	3-Heptanone	114	C7H14O	000106-35-4	16
5	3-Pentanone, 2,2,4,4-tetramethyl-	142	C9H18O	000815-24-7	12





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Operator : CG\JU
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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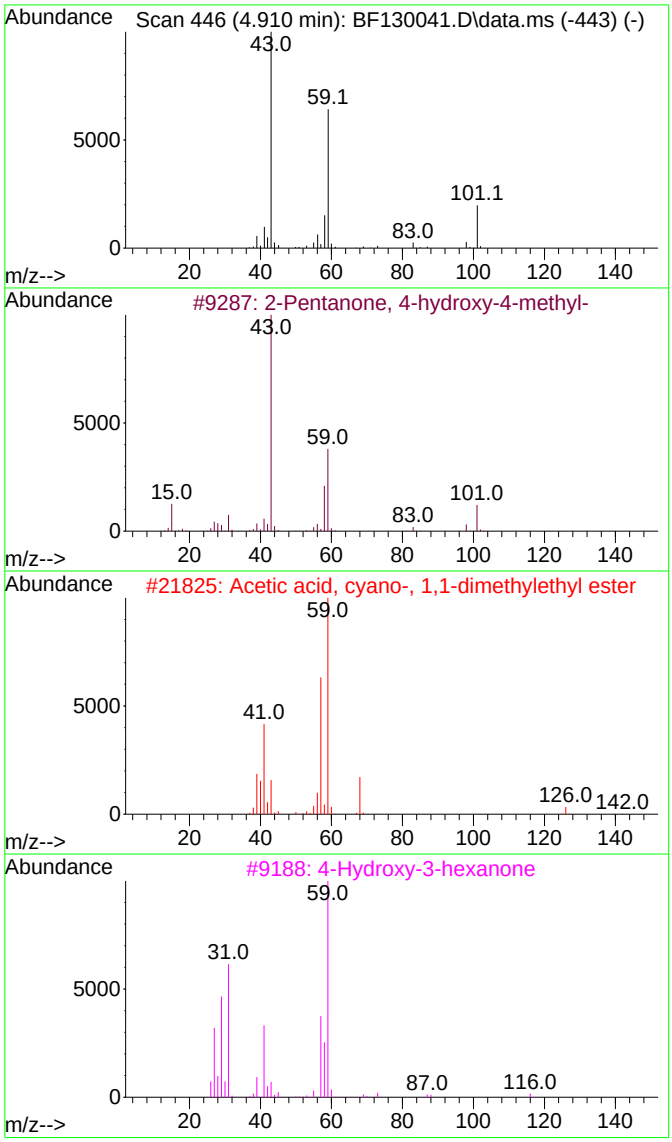
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

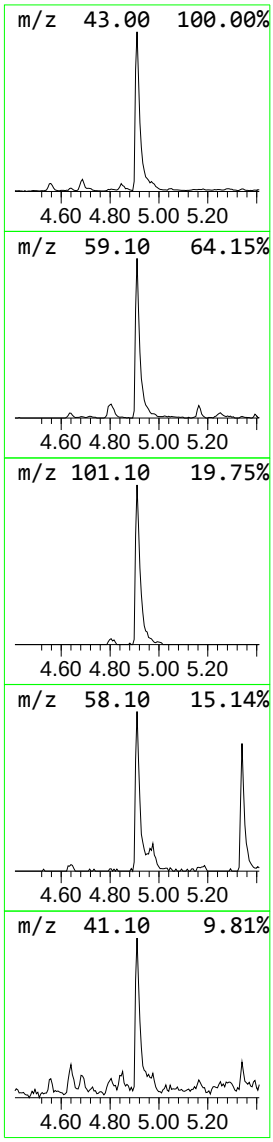
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	9.31 ng	318198	1,4-Dichlorobenzene-d4	6.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

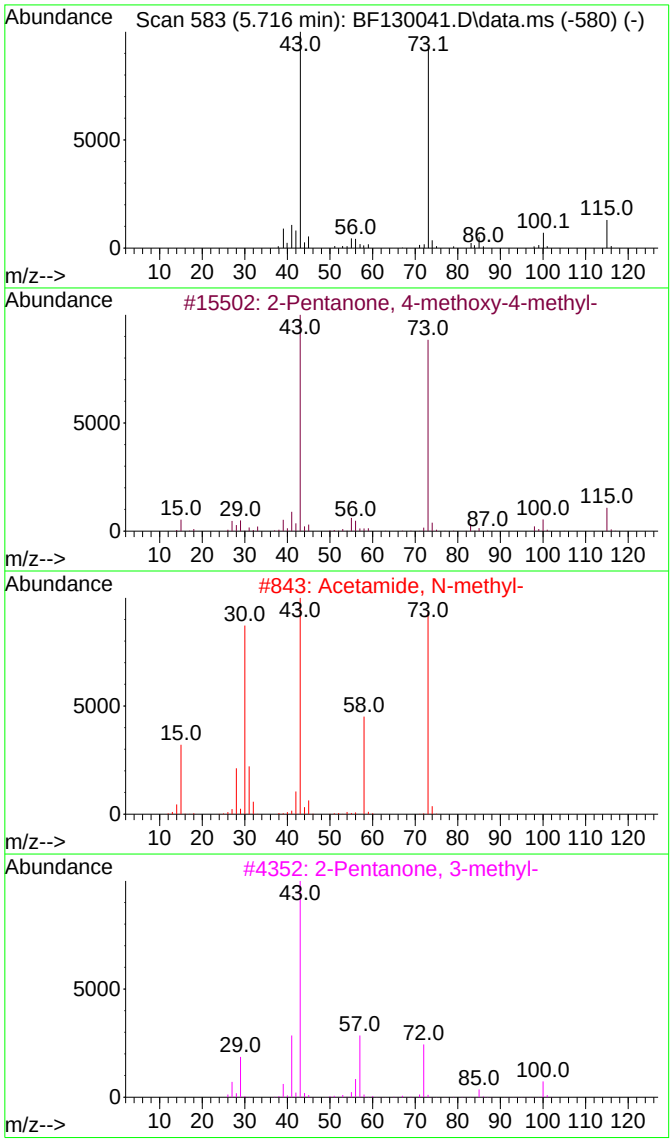
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

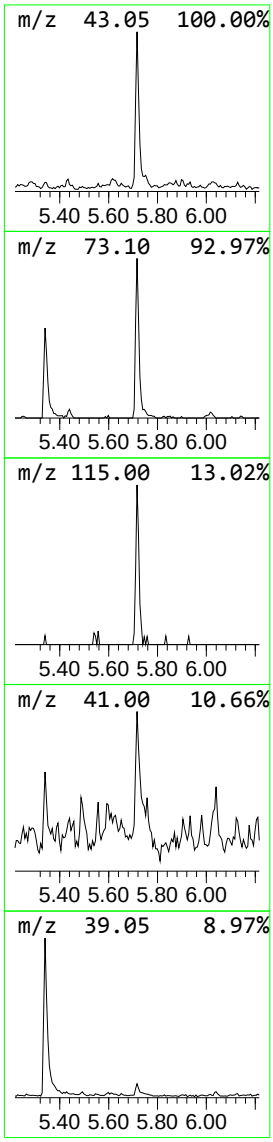
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.716	2.02 ng	69120	1,4-Dichlorobenzene-d4	6.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	49
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	27
4	Butane, 2,3-dimethoxy-2-methyl-	132	C7H16O2	074421-00-4	23
5	3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	16





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

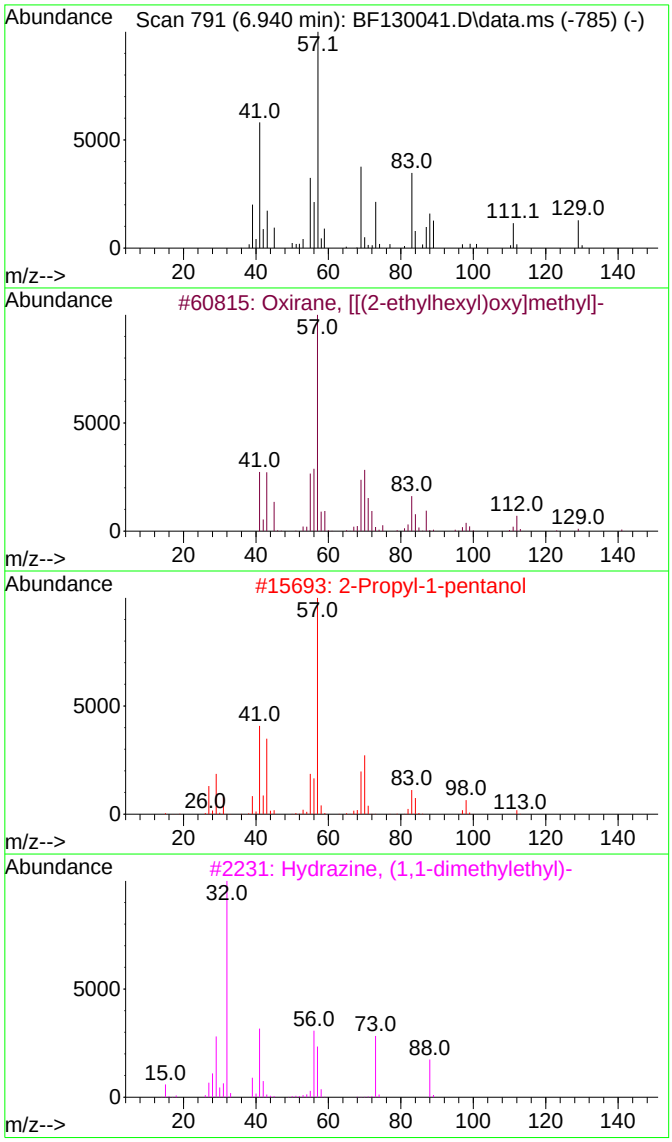
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

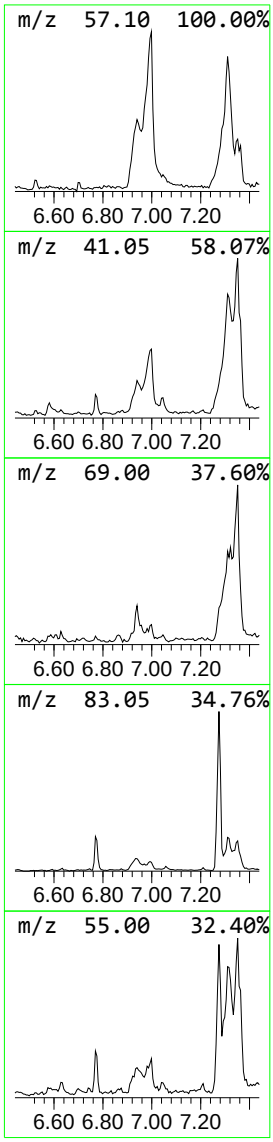
****

Peak Number 6 unknown6.940 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.940	3.58 ng	122395	1,4-Dichlorobenzene-d4	6.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	32
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	27
3	Hydrazine, (1,1-dimethylethyl)-	88	C4H12N2	032064-67-8	25
4	Oxirane, [(tetradecyloxy)methyl]-	270	C17H34O2	038954-75-5	25
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	25





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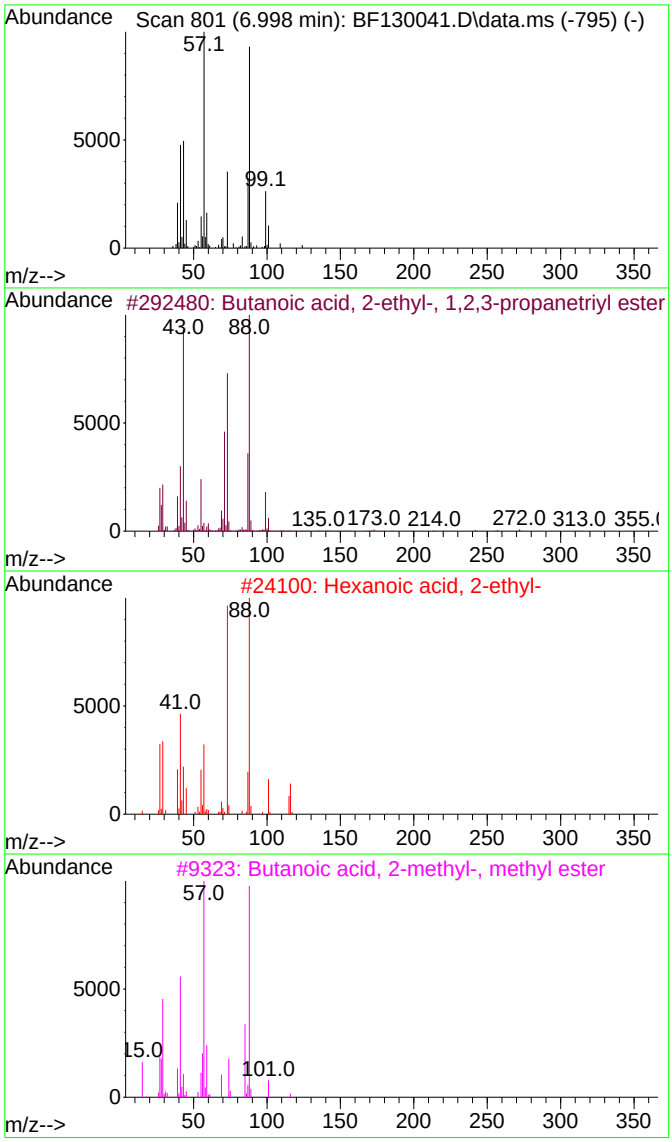
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

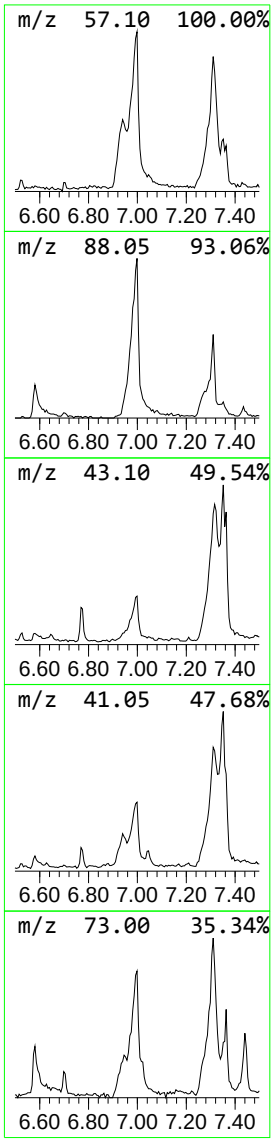
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butanoic acid, 2-ethyl-, 1,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.998	8.47 ng	289471	1,4-Dichlorobenzene-d4	6.698

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	64
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	38
3	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	33
4	Butanoic acid, 2-hydroxy-3,3-dim...	132	C6H12O3	004026-20-4	25
5	Butanoic acid, 2,2-diethyl-	144	C8H16O2	000813-58-1	25





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TIC Library : C:\Database\NIST20.L
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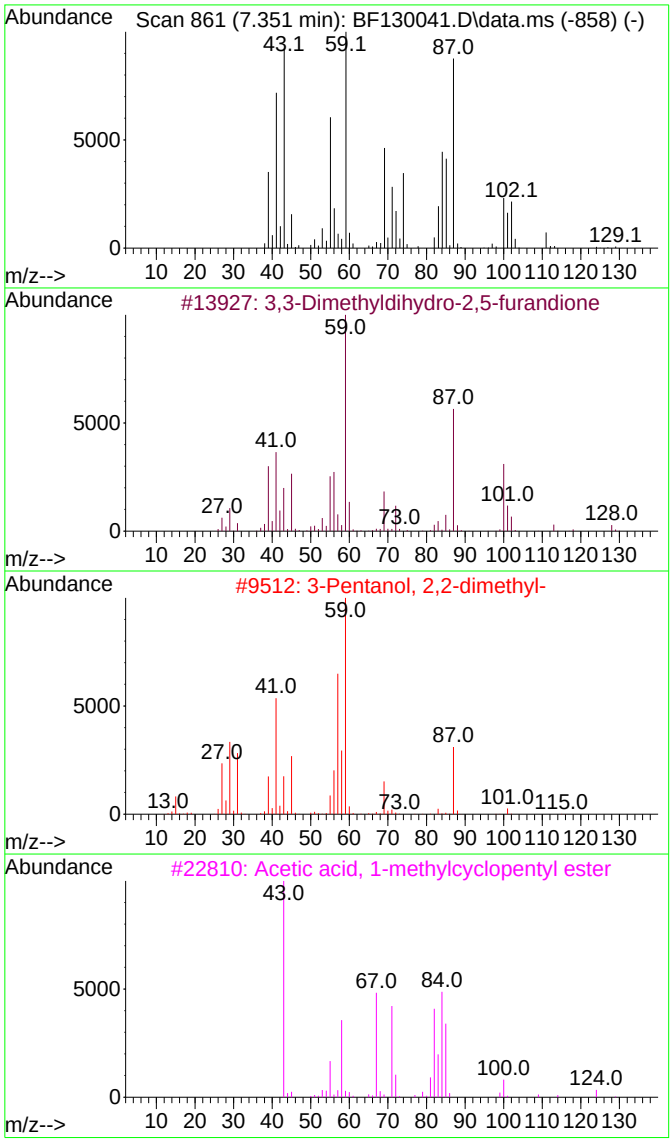
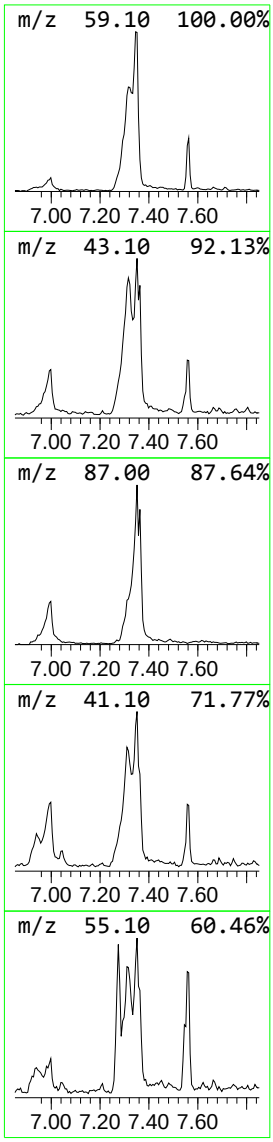
****

Peak Number 8 unknown7.351 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.351	11.54 ng	551934	Naphthalene-d8	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethyldihydro-2,5-furandione	128	C6H8O3	017347-61-4	43
2	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	38
3	Acetic acid, 1-methylcyclopentyl...	142	C8H14O2	026600-59-9	12
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	10
5	2-Pentene, 2-methoxy-	100	C6H12O	061142-47-0	10





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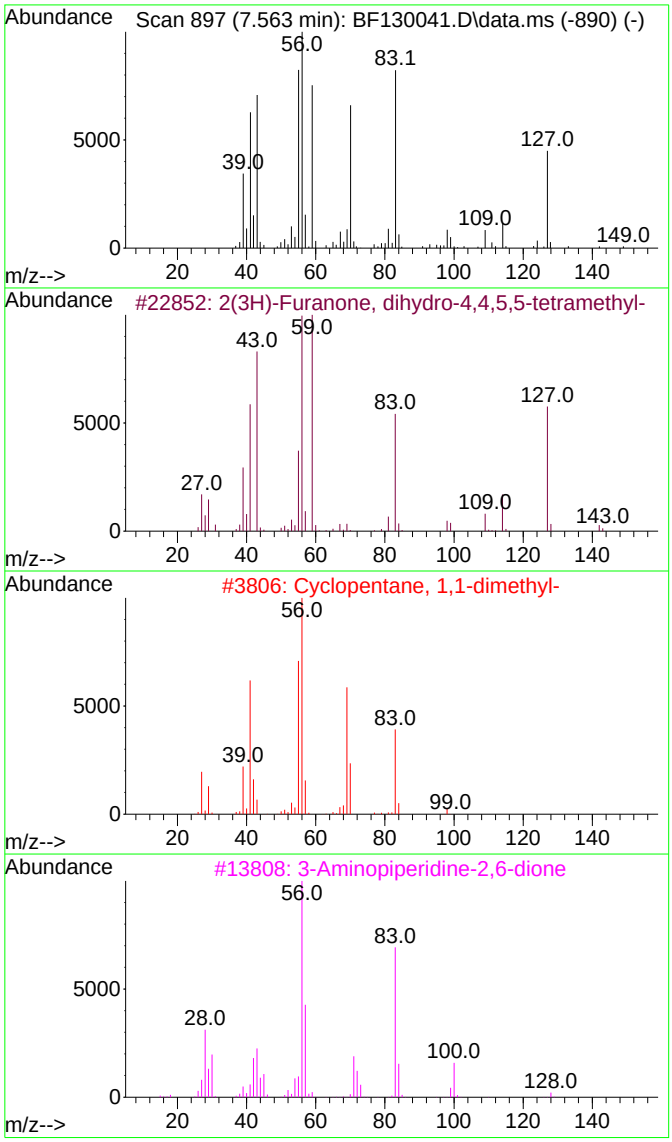
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

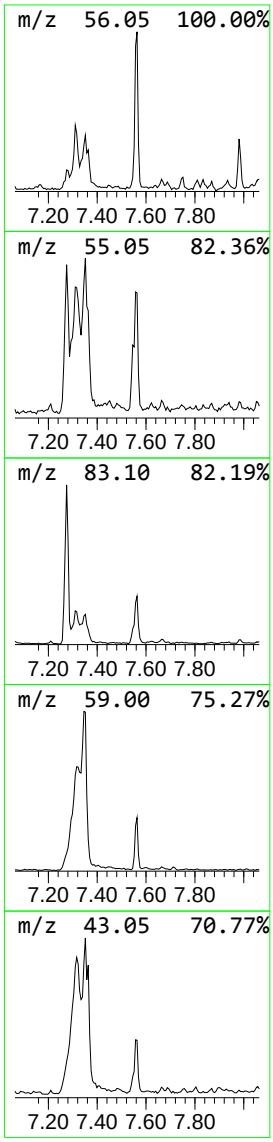
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 2(3H)-Furanone, dihydro-4,4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	4.62 ng	220976	Naphthalene-d8	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-4,4,5,5-...	142	C8H14O2	016466-24-3	50
2	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	49
3	3-Aminopiperidine-2,6-dione	128	C5H8N2O2	002353-44-8	35
4	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	22
5	2,4,4,6-Tetramethyl-[1,3,2]dioxa...	142	C7H15BO2	211613-23-9	22





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Data File : BF130041.D
Acq On : 29 Aug 2022 18:49
Operator : CG\JU
Sample : N4355-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

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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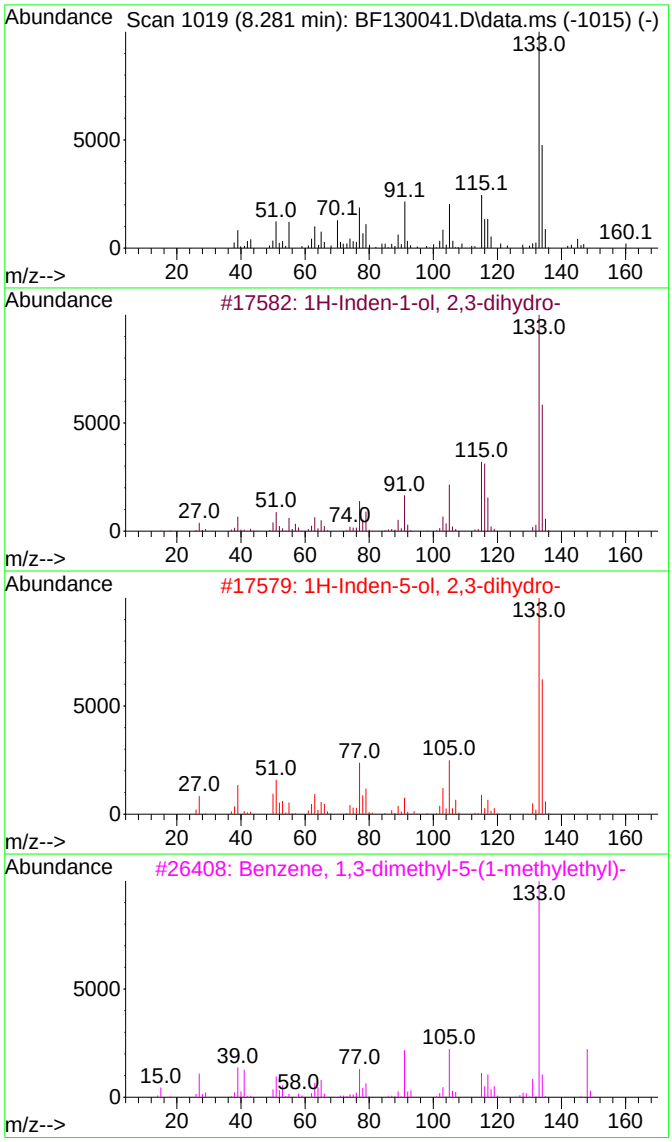
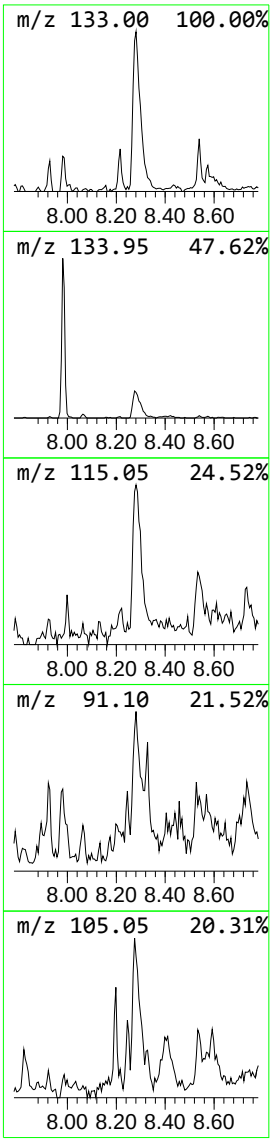
Peak Number 10 1H-Inden-1-ol, 2,3-dihydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.281	3.07 ng	146728	Naphthalene-d8	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-ol, 2,3-dihydro-	134	C9H10O	006351-10-6	90
2	1H-Inden-5-ol, 2,3-dihydro-	134	C9H10O	001470-94-6	76
3	Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	50
4	1-methyl-1-indanol	148	C10H12O	064666-42-8	50
5	Benzaldehyde, 2-ethyl-	134	C9H10O	022927-13-5	47





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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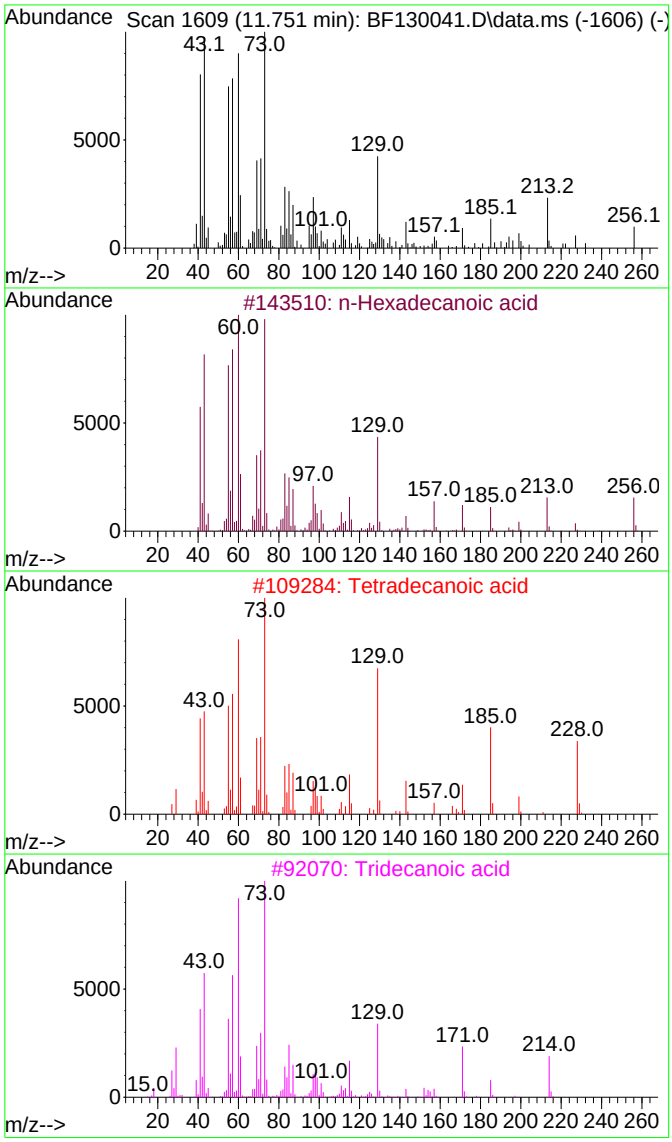
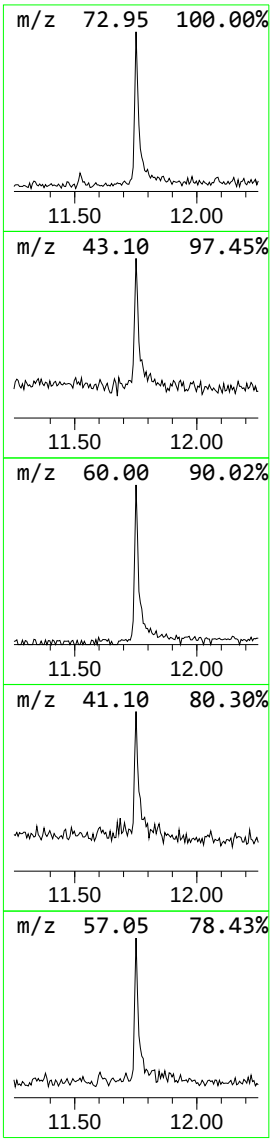
Peak Number 11 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.751	2.84 ng	132338	Phenanthrene-d10	11.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





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Data File : BF130041.D
Acq On : 29 Aug 2022 18:49
Operator : CG\JU
Sample : N4355-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

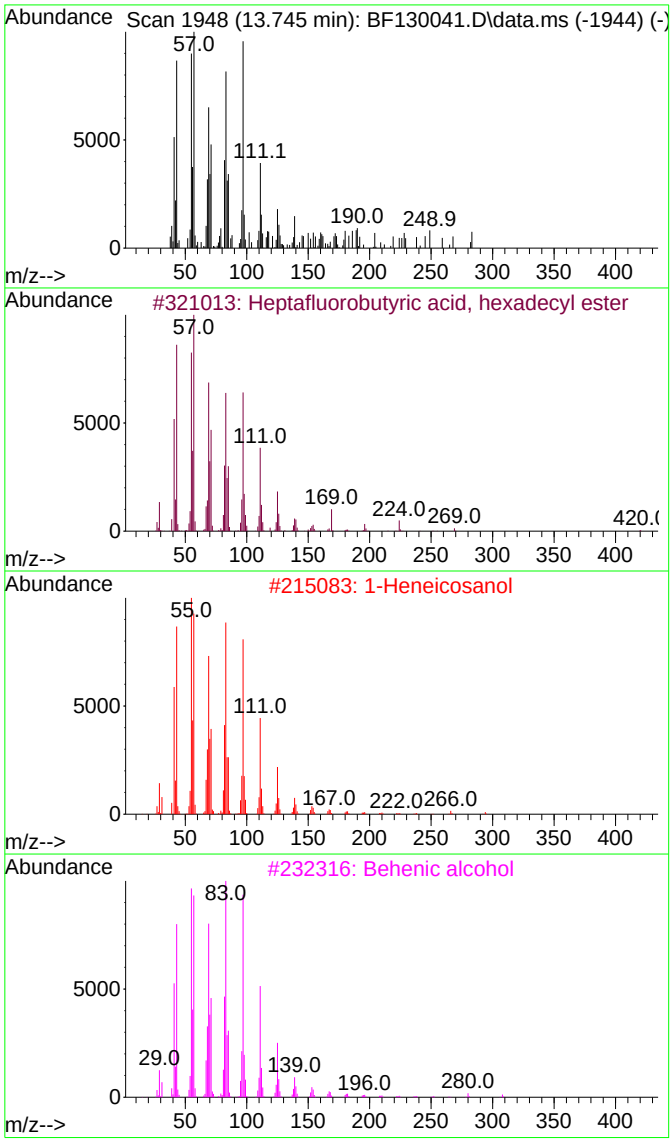
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

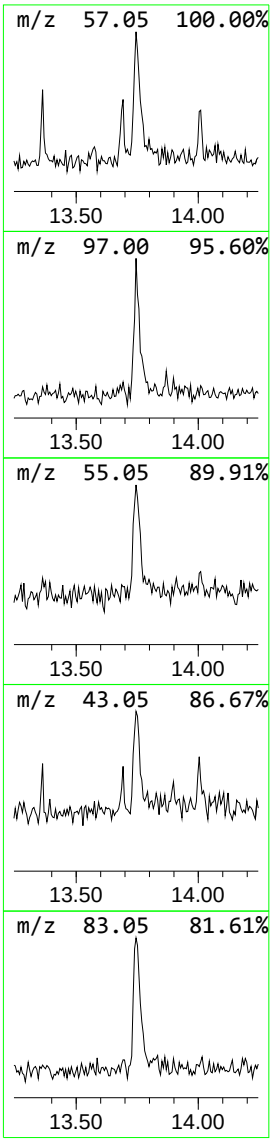
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Heptafluorobutyric acid, he... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	2.77 ng	76140	Chrysene-d12	13.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	87





Tentatively Identified Compound (LSC) summary

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Data File : BF130041.D
Acq On : 29 Aug 2022 18:49
Operator : CG\JU
Sample : N4355-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-34

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Butanol, 2,3-...	2.875	4.8	ng	165421	1	6.698	683383	20.0
1-Ethoxypentan-...	4.157	4.2	ng	144800	1	6.698	683383	20.0
unknown4.252	4.252	5.2	ng	177195	1	6.698	683383	20.0
2-Pentanone, 4-...	4.910	9.3	ng	318198	1	6.698	683383	20.0
2-Pentanone, 4-...	5.716	2.0	ng	69120	1	6.698	683383	20.0
unknown6.940	6.940	3.6	ng	122395	1	6.698	683383	20.0
Butanoic acid, ...	6.998	8.5	ng	289471	1	6.698	683383	20.0
unknown7.351	7.351	11.5	ng	551934	2	7.981	956760	20.0
2(3H)-Furanone,...	7.563	4.6	ng	220976	2	7.981	956760	20.0
1H-Inden-1-ol, ...	8.281	3.1	ng	146728	2	7.981	956760	20.0
n-Hexadecanoic ...	11.751	2.8	ng	132338	4	11.222	931717	20.0
Heptafluorobuty...	13.745	2.8	ng	76140	5	13.869	548999	20.0