LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132026.D
Acq On : 11 Jan 2023 16:51
Operator : CG\JU
Sample : 01072-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
H-5-MIDDLE(4-8)

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-BF010923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132026.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.334	378	382	387	rBV	29743	35124	1.25%	0.197%
2	4.987	486	493	496	rBV	862839	1072422	38.15%	6.024%
3	5.398	559	563	576	rVB	1215504	1108996	39.45%	6.229%
4	6.428	733	738	751	rBV	2042906	1984654	70.61%	11.148%
5	6.775	794	797	801	rBV	560094	487175	17.33%	2.737%
6	7.351	889	895	898	rBV	1439080	1401566	49.86%	7.873%
7	8.069	1012	1017	1020	rBV	714466	639107	22.74%	3.590%
8	9.151	1195	1201	1204	rBV	3095322	2810893	100.00%	15.789%
9	9.828	1308	1316	1320	rBV	883835	757787	26.96%	4.257%
10	10.545	1434	1438	1442	rVB	425353	343373	12.22%	1.929%
11	10.622	1448	1451	1455	rBV	92592	74772	2.66%	0.420%
12	10.998	1507	1515	1519	rVV	50932	79194	2.82%	0.445%
13	11.039	1519	1522	1527	rVB	84590	70359	2.50%	0.395%
14	11.322	1564	1570	1573	rBV	971085	802818	28.56%	4.509%
15	11.851	1654	1660	1663	rBV4	37639	58621	2.09%	0.329%
16	11.998	1682	1685	1689	rBV2	45819	61830	2.20%	0.347%
17	12.039	1689	1692	1699	rVB2	59080	92366	3.29%	0.519%
18	12.733	1807	1810	1814	rBV	71211	60171	2.14%	0.338%
19	12.916	1836	1841	1845	rBV	2618857	2666420	94.86%	14.978%
20	13.404	1917	1924	1931	rBV	1781762	1987489	70.71%	11.164%
21	13.474	1933	1936	1940	rVV2	37639	42378	1.51%	0.238%
22	13.821	1991	1995	2002	rBV	152198	233439	8.30%	1.311%
23	13.974	2017	2021	2025	rBV	477346	408185	14.52%	2.293%
24	15.033	2194	2201	2206	rBV10	49602	145947	5.19%	0.820%
25	15.439	2266	2270	2277	rBV	299327	377746	13.44%	2.122%

Sum of corrected areas: 17802832

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Misc :
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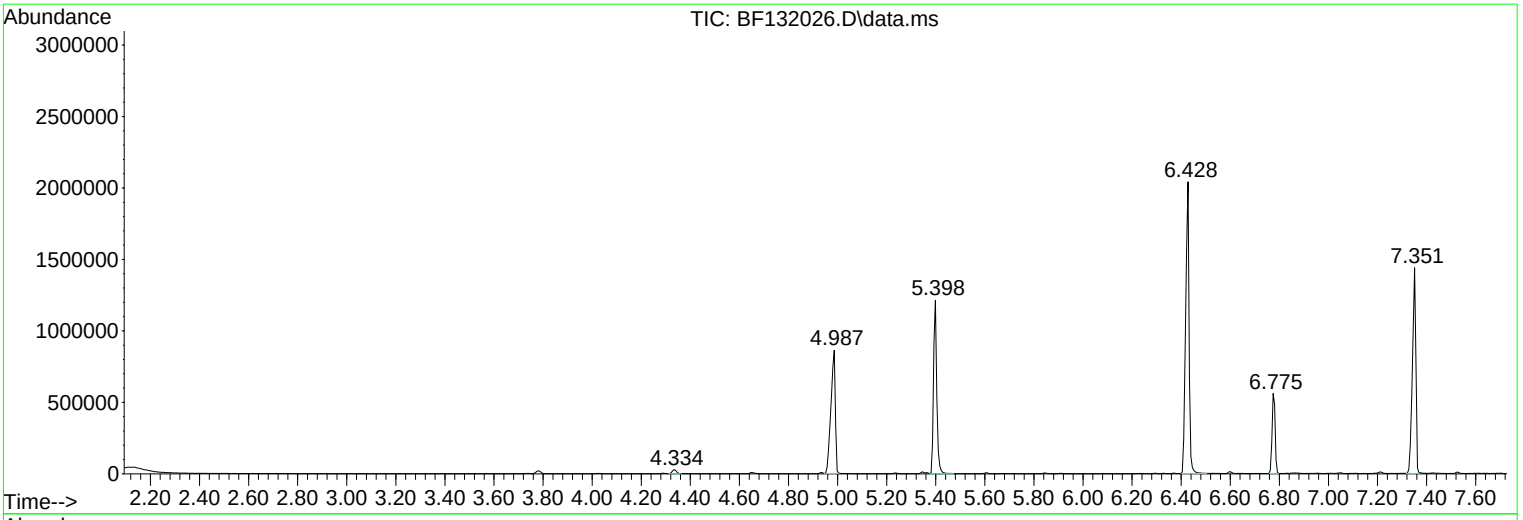
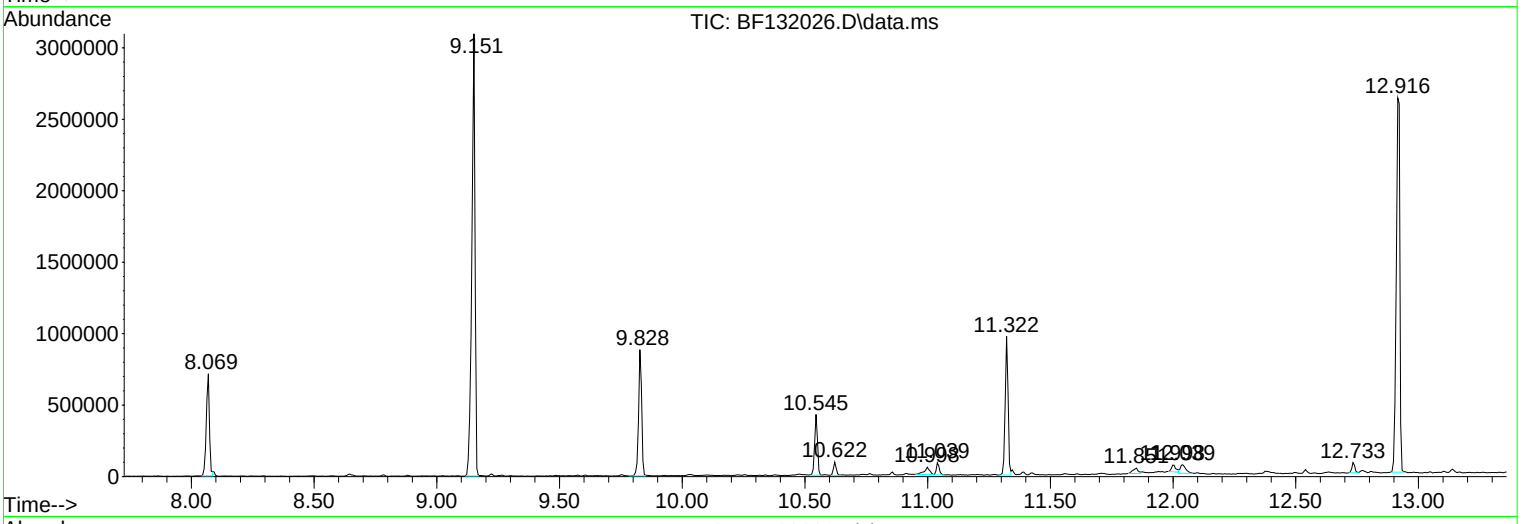
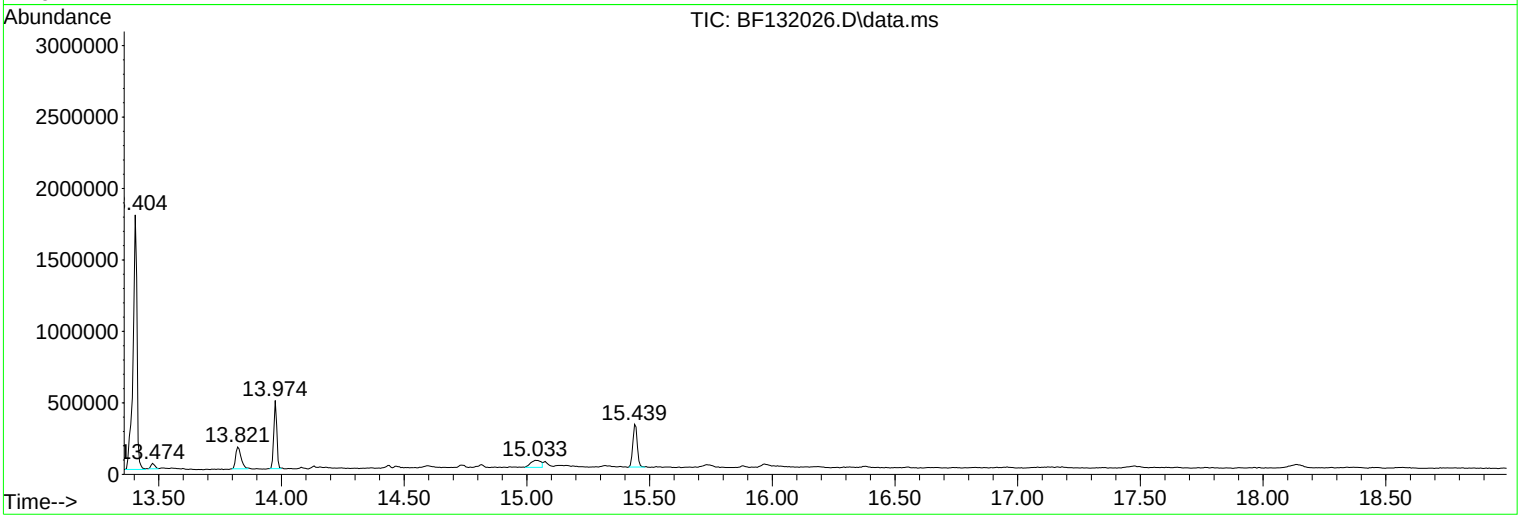
Instrument :
BNA_F
ClientSampleId :
H-5-MIDDLE(4-8)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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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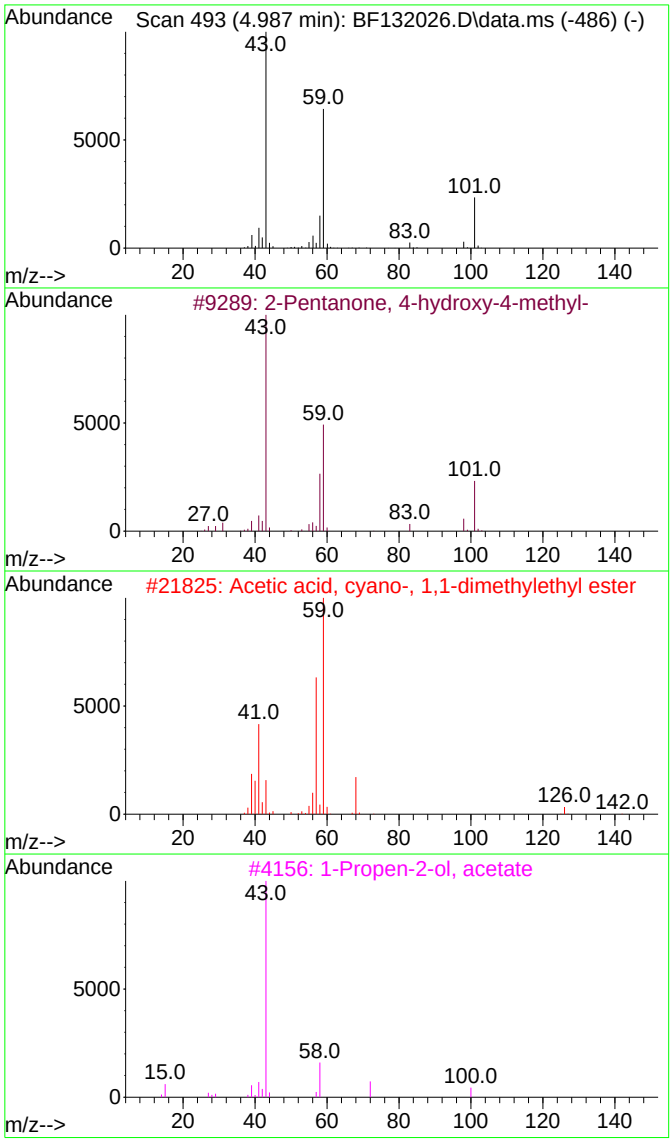
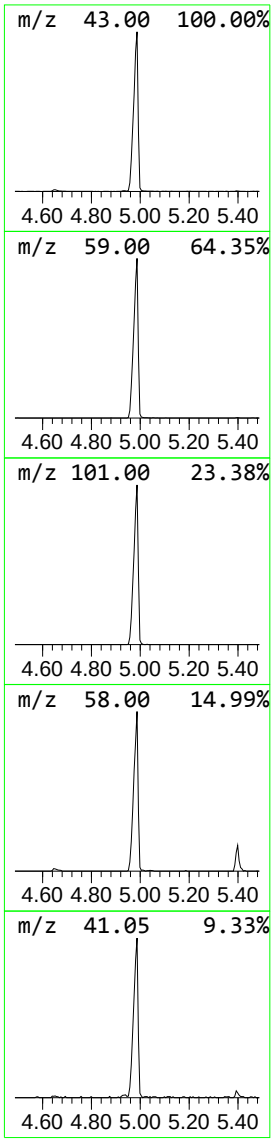
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	44.03 ng	1072420	1,4-Dichlorobenzene-d4	6.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument :
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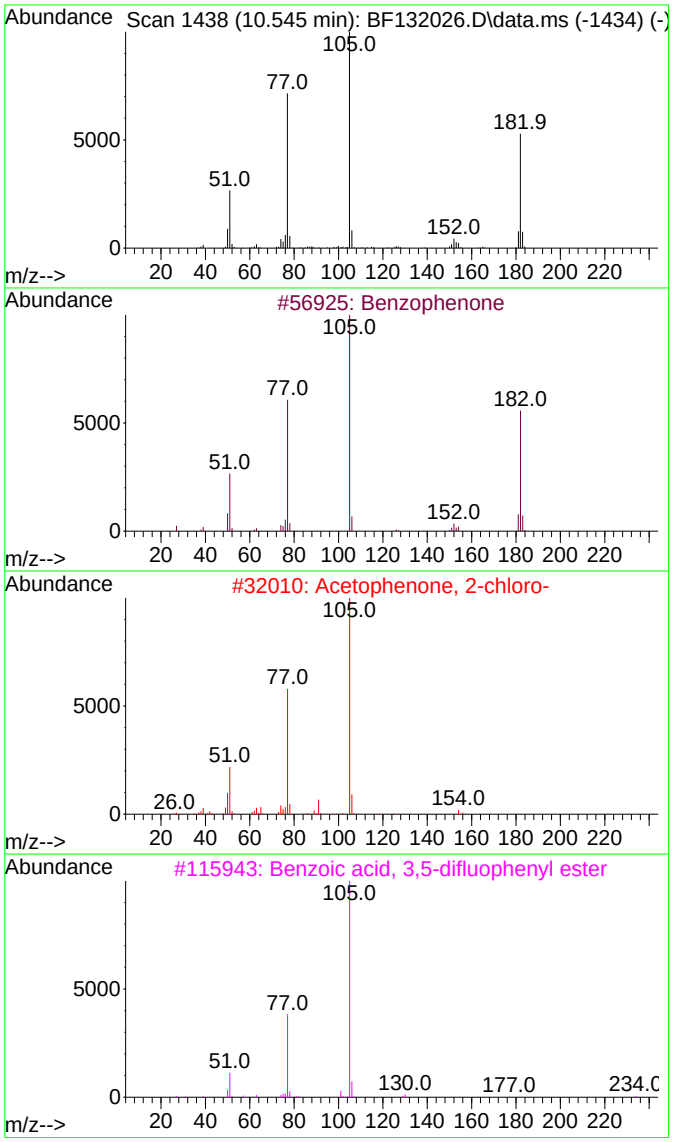
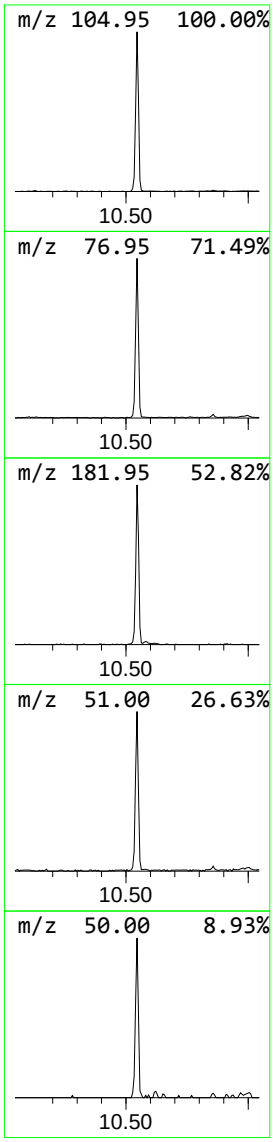
****

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.545	9.06 ng	343373	Acenaphthene-d10	9.828

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	49
3	Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	47
4	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47





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H-5-MIDDLE(4-8)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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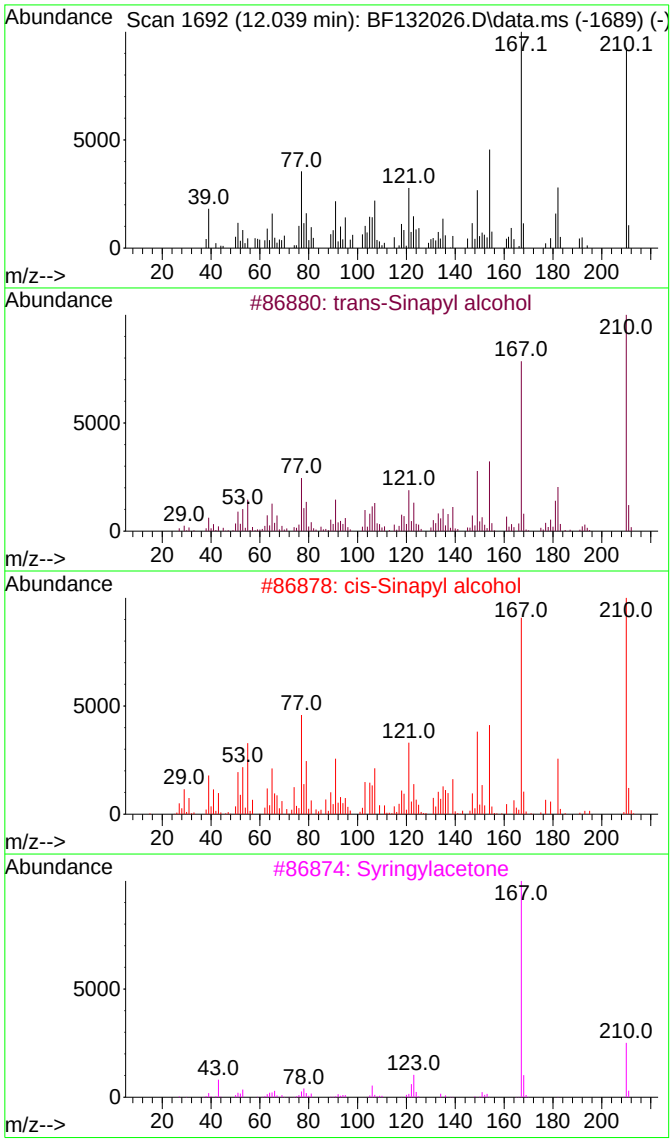
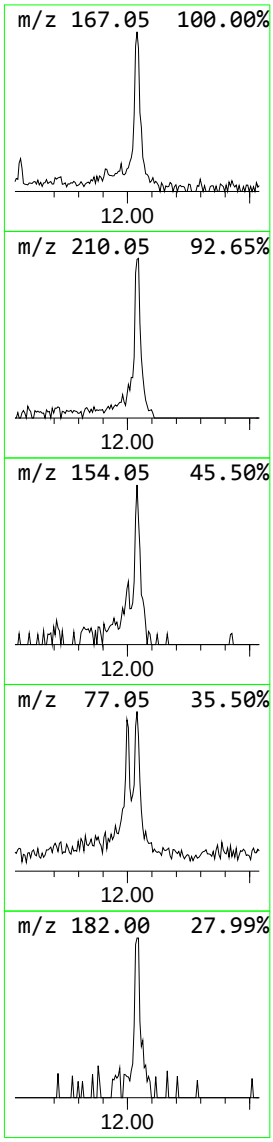
****

Peak Number 3 trans-Sinapyl alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	2.30 ng	92366	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	91
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	83
3	Syringylacetone	210	C11H14O4	019037-58-2	60
4	2-methyl-3-(phenylethynyl)cycloh...	210	C15H14O	1010466-55-6	47
5	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	41





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
H-5-MIDDLE(4-8)

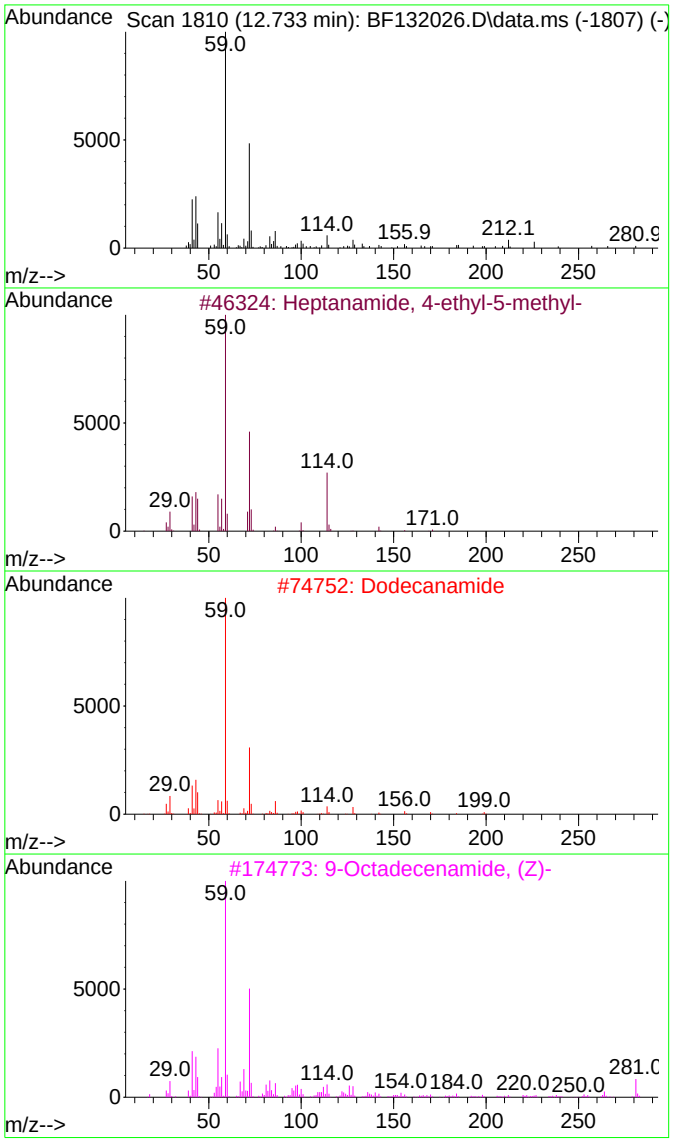
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

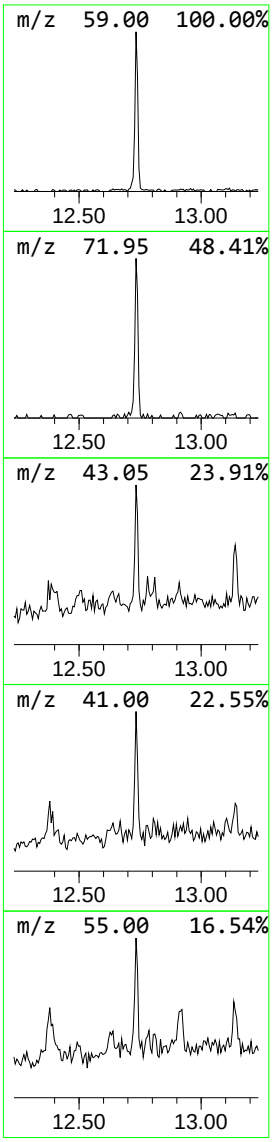
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heptanamide, 4-ethyl-5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.95 ng	60171	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	83
2	Dodecanamide	199	C12H25NO	001120-16-7	81
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
4	Nonanamide	157	C9H19NO	001120-07-6	72
5	Hexadecanamide	255	C16H33NO	000629-54-9	64





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Sample : 01072-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
H-5-MIDDLE(4-8)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

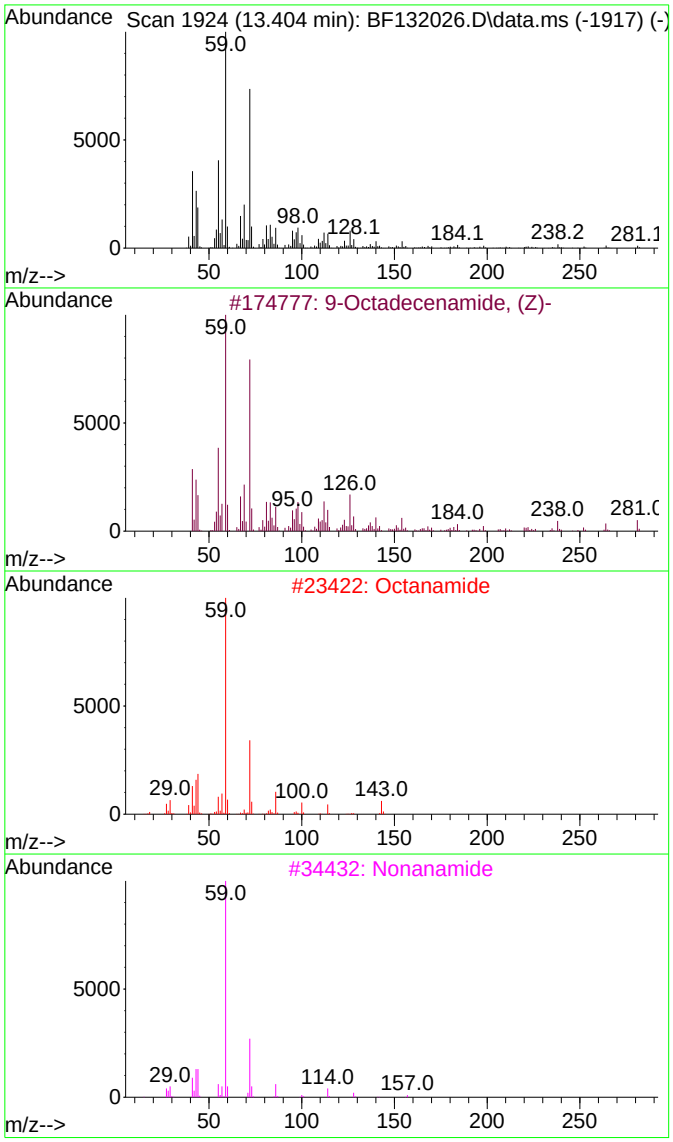
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

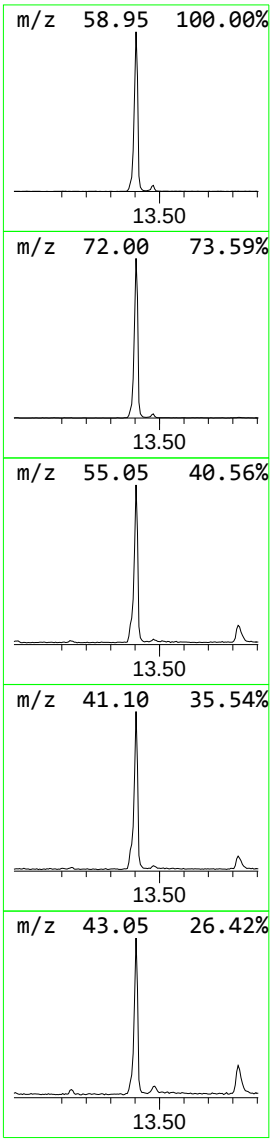
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.404	97.38 ng	1987490	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Octanamide	143	C8H17NO	000629-01-6	47
3	Nonanamide	157	C9H19NO	001120-07-6	47
4	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	47
5	Dodecanamide	199	C12H25NO	001120-16-7	47





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H-5-MIDDLE(4-8)

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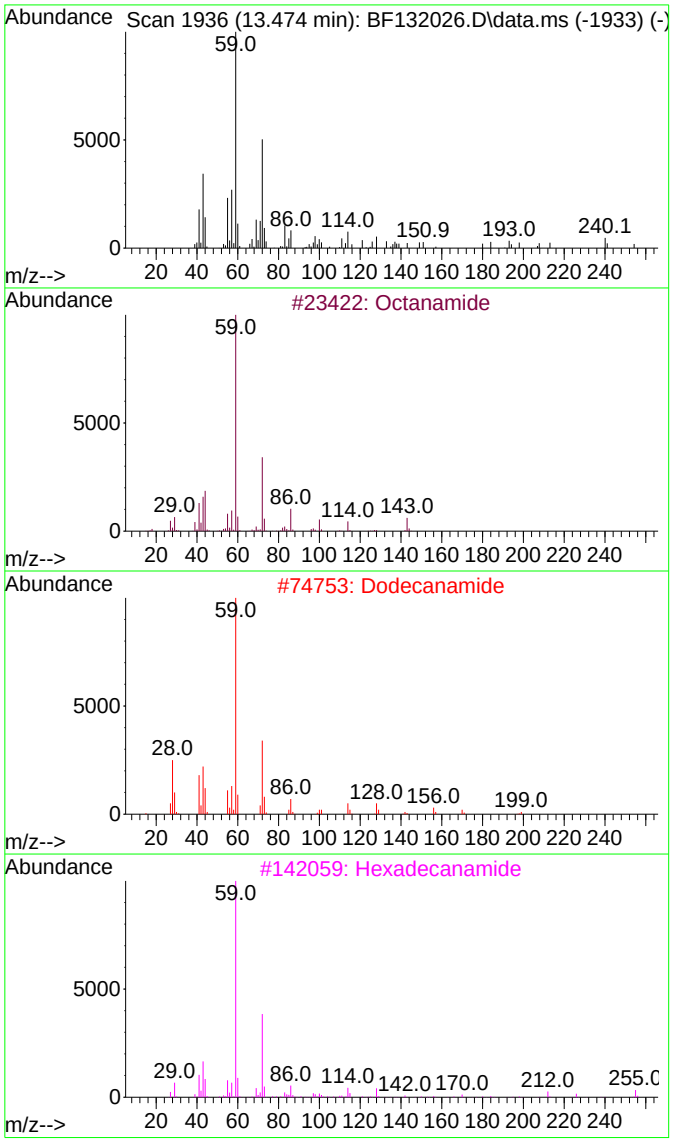
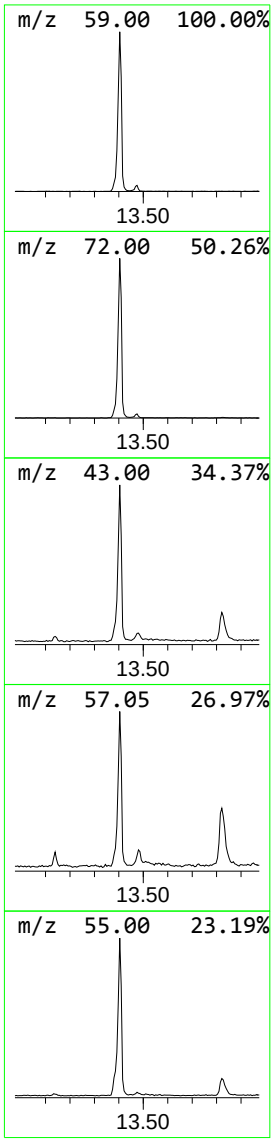
Peak Number 6 Octanamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	2.08 ng	42378	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanamide	143	C8H17NO	000629-01-6	78
2	Dodecanamide	199	C12H25NO	001120-16-7	78
3	Hexadecanamide	255	C16H33NO	000629-54-9	78
4	Tetradecanamide	227	C14H29NO	000638-58-4	64
5	Octadecanamide	283	C18H37NO	000124-26-5	64





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ClientSampleId :
H-5-MIDDLE(4-8)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

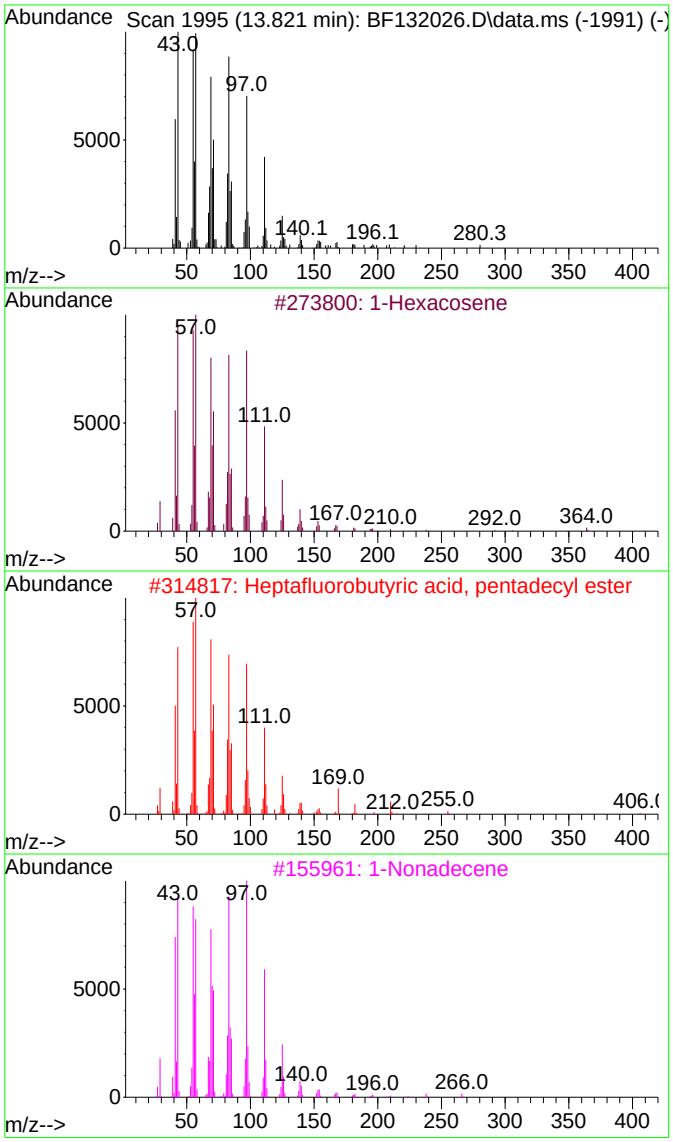
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

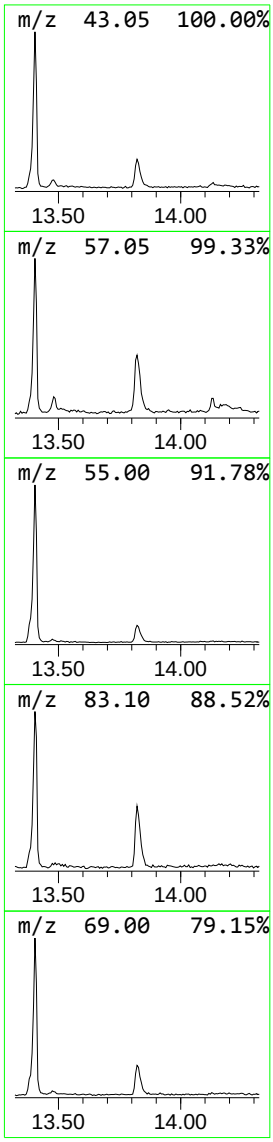
****

Peak Number 7 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	11.44 ng	233439	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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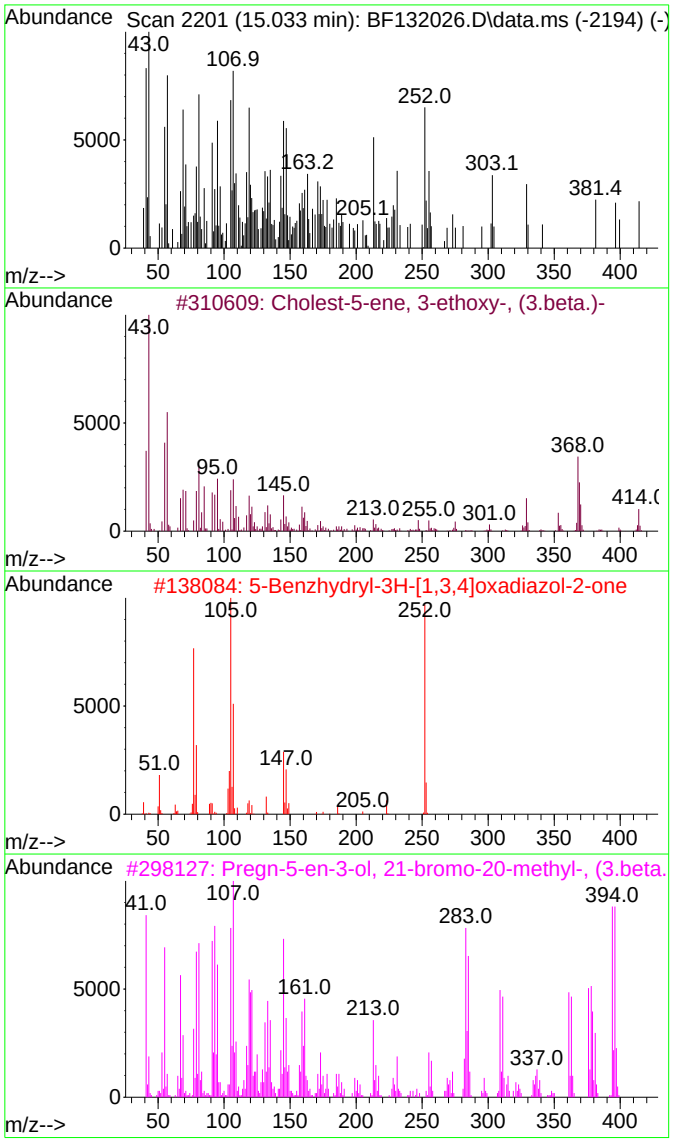
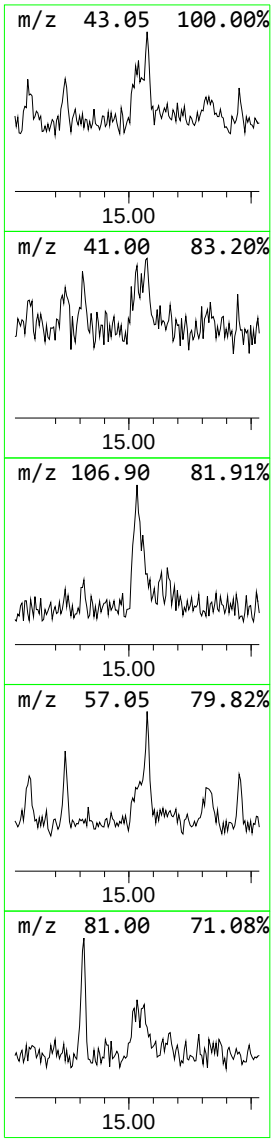
****

Peak Number 8 unknown15.033 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.033	7.73 ng	145947	Perylene-d12	15.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	35
2	5-Benzhydryl-3H-[1,3,4]oxadiazol...	252	C15H12N2O2	1000318-50-4	27
3	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	27
4	Phenol, 4,4'-(3-ethenyl-1-propen...	252	C17H16O2	017676-24-3	16
5	Stigmasta-3,5-diene	396	C29H48	004970-37-0	14





Tentatively Identified Compound (LSC) summary

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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-Pentanone, 4-...	4.987	44.0	ng	1072420	1	6.775	487175	20.0
Benzophenone	10.545	9.1	ng	343373	3	9.828	757787	20.0
trans-Sinapyl a...	12.039	2.3	ng	92366	4	11.322	802818	20.0
Heptanamide, 4-...	12.733	3.0	ng	60171	5	13.974	408185	20.0
9-Octadecenamid...	13.404	97.4	ng	1987490	5	13.974	408185	20.0
Octanamide	13.474	2.1	ng	42378	5	13.974	408185	20.0
1-Hexacosene	13.821	11.4	ng	233439	5	13.974	408185	20.0
unknown15.033	15.033	7.7	ng	145947	6	15.439	377746	20.0