LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124802.D
Acq On : 27 Jul 2021 19:51
Operator : JU/CG
Sample : M3165-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-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-BF072221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124802.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	11	rBB2	10708	12142	3.86%	0.752%
2	5.487	573	578	581	rBB	176453	165948	52.70%	10.274%
3	6.498	745	750	753	rBB	167326	168158	53.40%	10.411%
4	6.869	810	813	816	rBB	37768	26916	8.55%	1.666%
5	7.433	905	909	912	rBB	121473	112471	35.72%	6.964%
6	8.051	1011	1014	1019	rBB	25071	18115	5.75%	1.122%
7	8.151	1028	1031	1034	rBB	50334	38171	12.12%	2.363%
8	9.227	1210	1214	1217	rBV	247408	229041	72.74%	14.181%
9	9.910	1327	1330	1333	rBB	61139	47465	15.07%	2.939%
10	10.698	1460	1464	1467	rBV	184757	163672	51.98%	10.134%
11	11.398	1579	1583	1586	rBB	61898	54817	17.41%	3.394%
12	11.916	1669	1671	1673	rBB	8293	5927	1.88%	0.367%
13	12.986	1848	1853	1856	rBV	341056	314877	100.00%	19.495%
14	13.545	1946	1948	1951	rBB	5880	4829	1.53%	0.299%
15	13.874	2002	2004	2012	rBB2	22064	25923	8.23%	1.605%
16	14.033	2028	2031	2034	rBV	60316	48318	15.35%	2.992%
17	14.192	2055	2058	2061	rBB	16546	12684	4.03%	0.785%
18	14.498	2107	2110	2113	rBB	17268	12925	4.10%	0.800%
19	14.792	2156	2160	2166	rBB2	71900	84747	26.91%	5.247%
20	15.145	2216	2220	2224	rBB	10880	12451	3.95%	0.771%
21	15.509	2277	2282	2289	rBB3	30675	44953	14.28%	2.783%
22	15.968	2356	2360	2364	rBB	4842	6596	2.09%	0.408%
23	16.486	2442	2448	2451	rBB	2621	4001	1.27%	0.248%

Sum of corrected areas: 1615147

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
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Misc :
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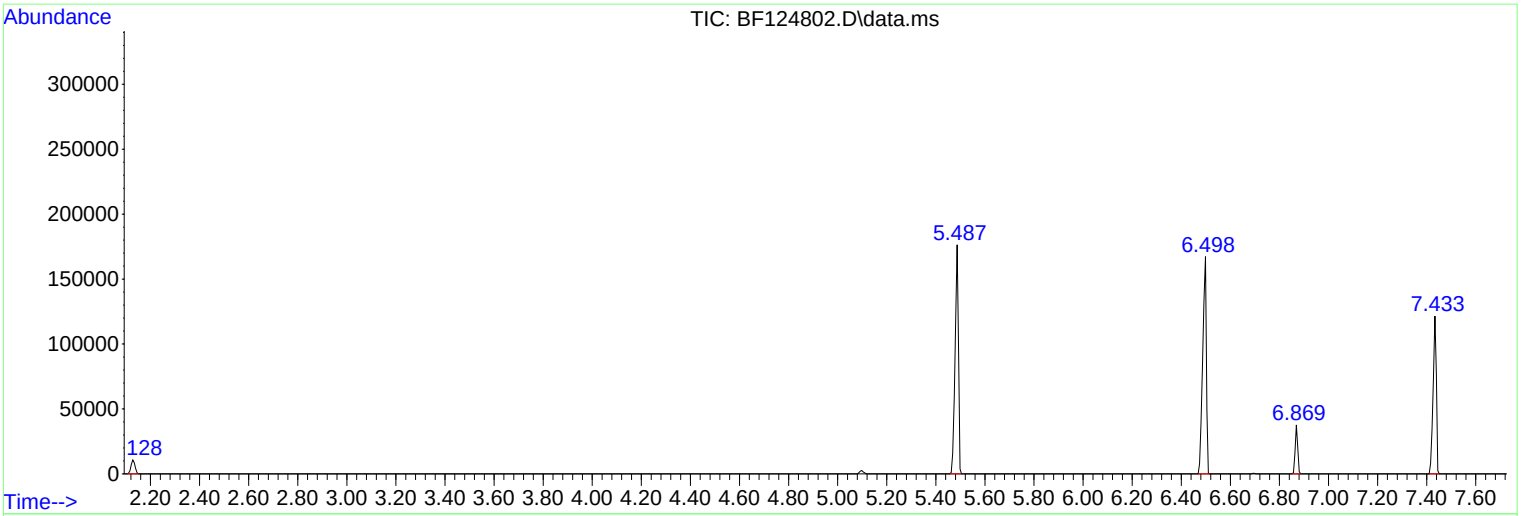
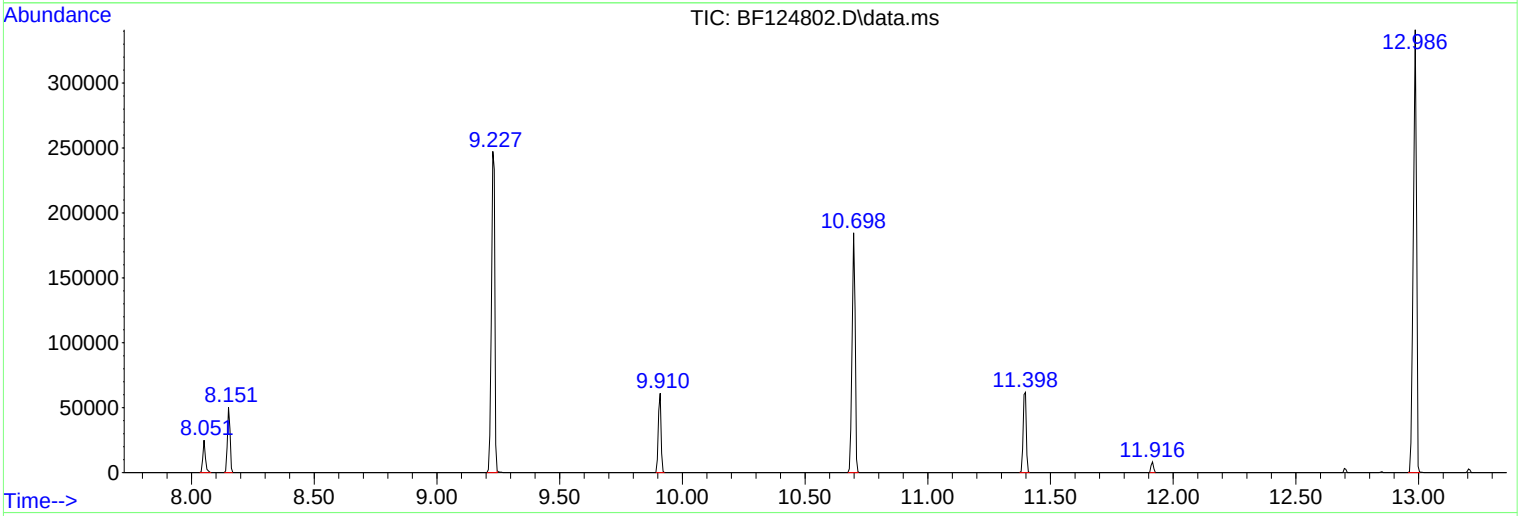
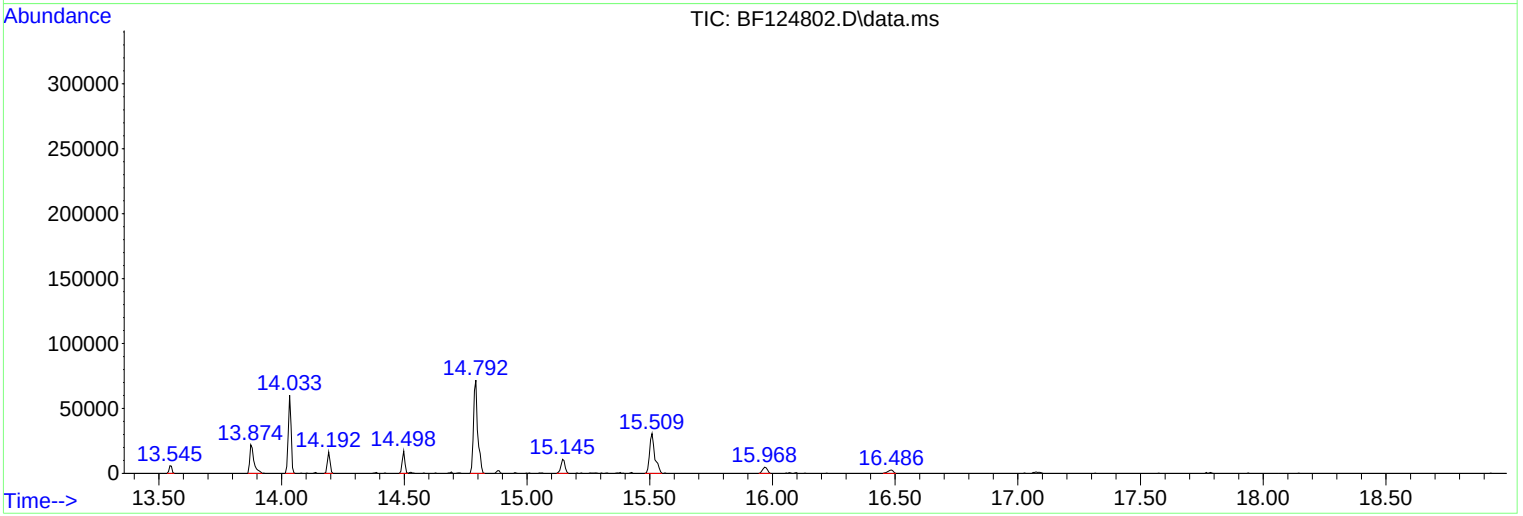
Instrument :
BNA_F
ClientSampleId :
COMP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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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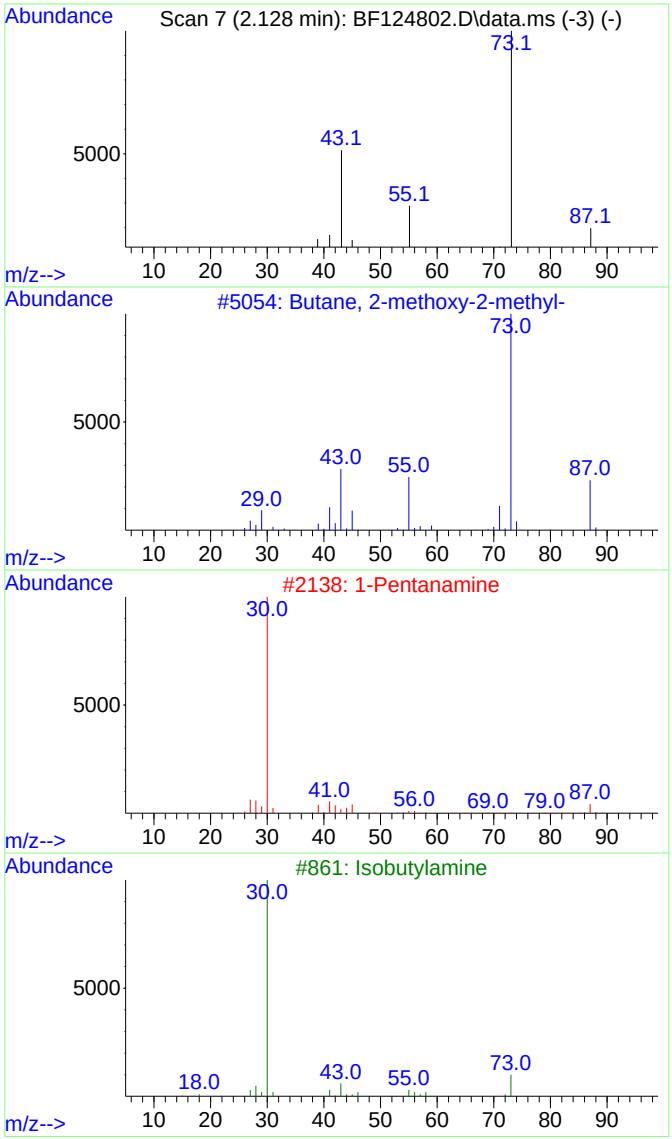
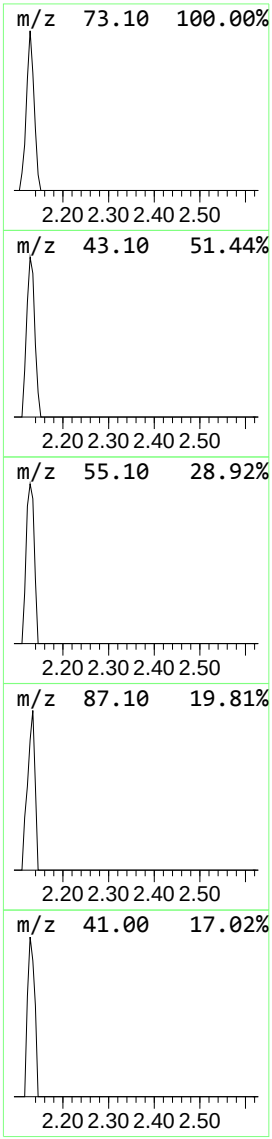
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	9.02 ng	12142	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2	1-Pentanamine	87	C5H13N	000110-58-7	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	4
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4





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Operator : JU/CG
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Instrument : BNA_F
ClientSampleId : COMP-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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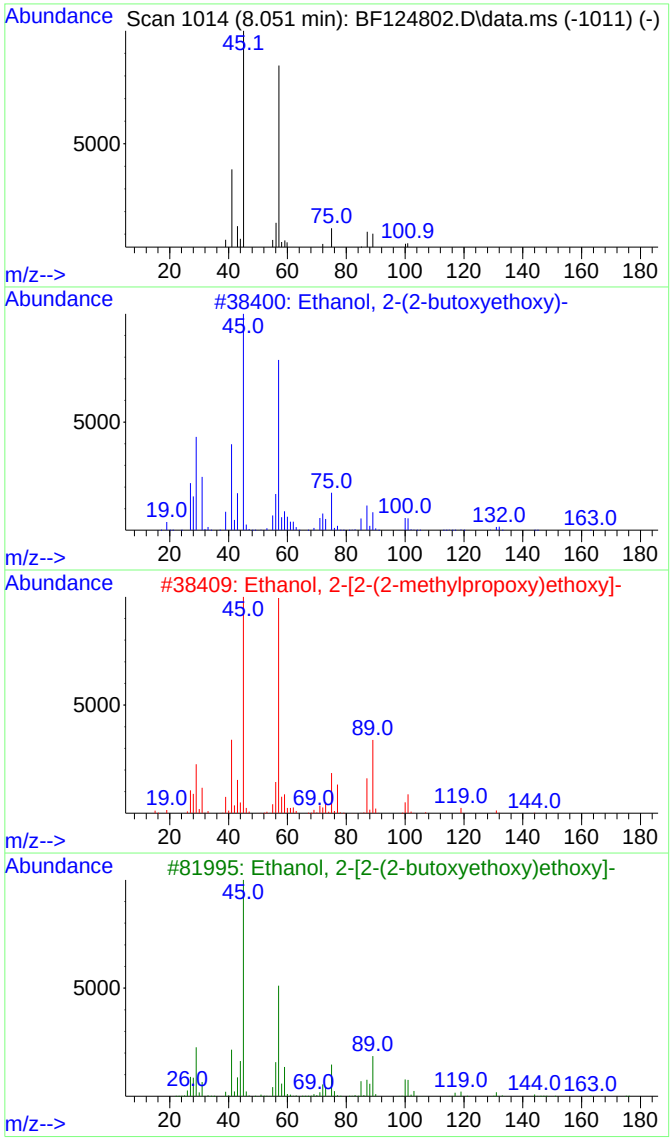
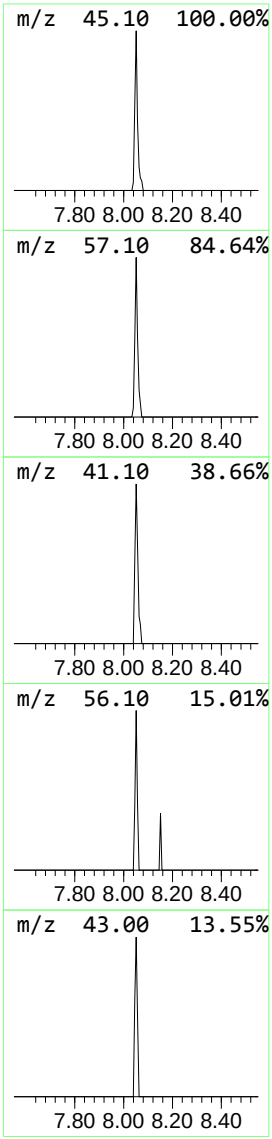
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	9.49 ng	18115	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	43
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	42
5	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40





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Sample : M3165-02
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Instrument :
BNA_F
ClientSampleId :
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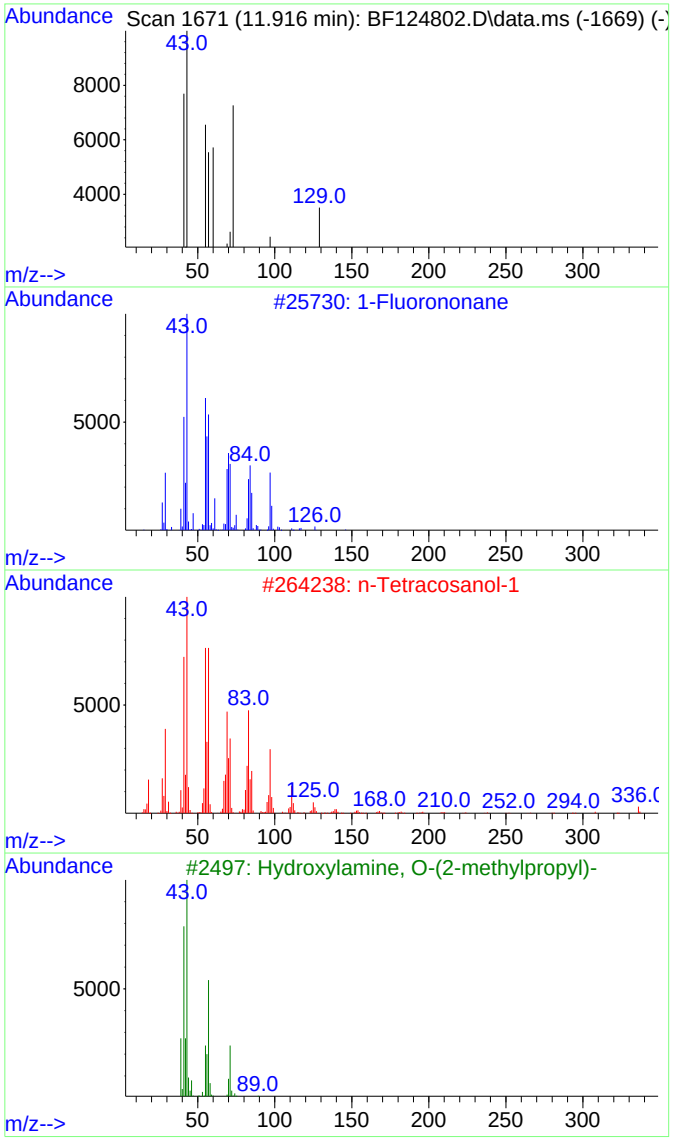
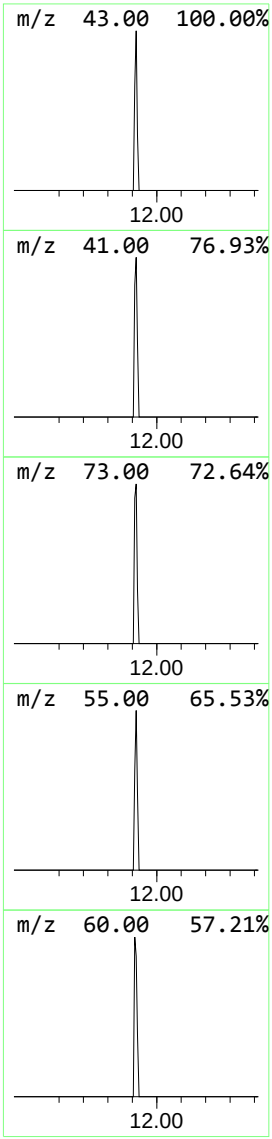
****

Peak Number 3 unknown11.916 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.16 ng	5927	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Fluorononane	146	C9H19F	000463-18-3	23
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	10
3	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	10
4	Cetene	224	C16H32	000629-73-2	9
5	Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	9





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Instrument : BNA_F
ClientSampleId : COMP-2

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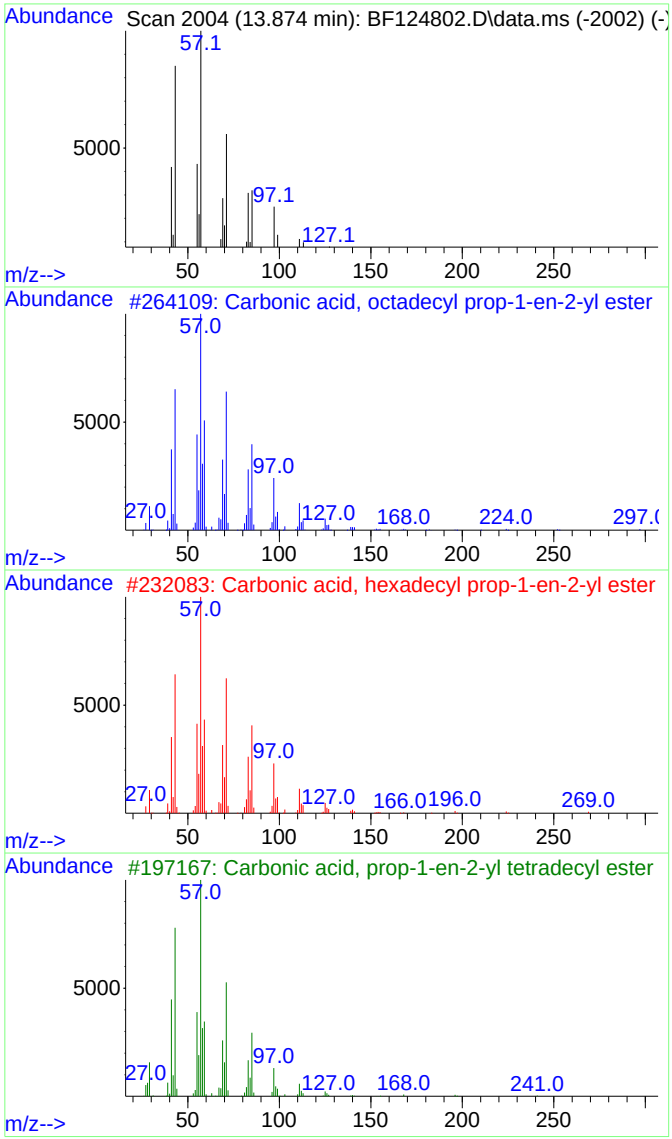
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

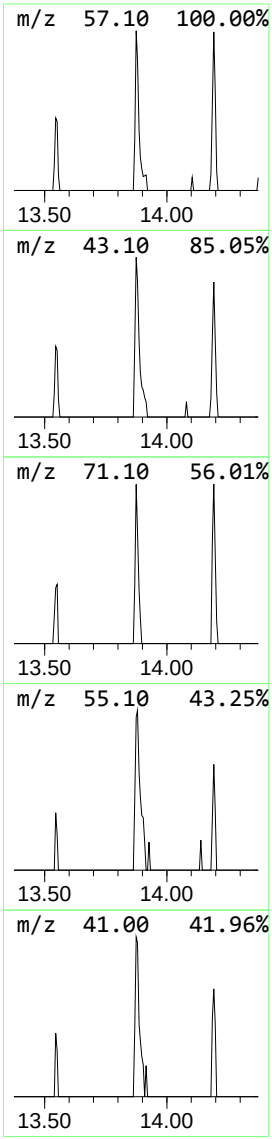
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Carbonic acid, octadecyl pr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	10.73 ng	25923	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	86
3	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	64
4	Eicosyl isobutyl ether	354	C24H50O	1000406-33-0	64
5	Isobutyl hexadecyl ether	298	C20H42O	1000406-32-8	59





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Operator : JU/CG
Sample : M3165-02
Misc :
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Instrument : BNA_F
ClientSampleId : COMP-2

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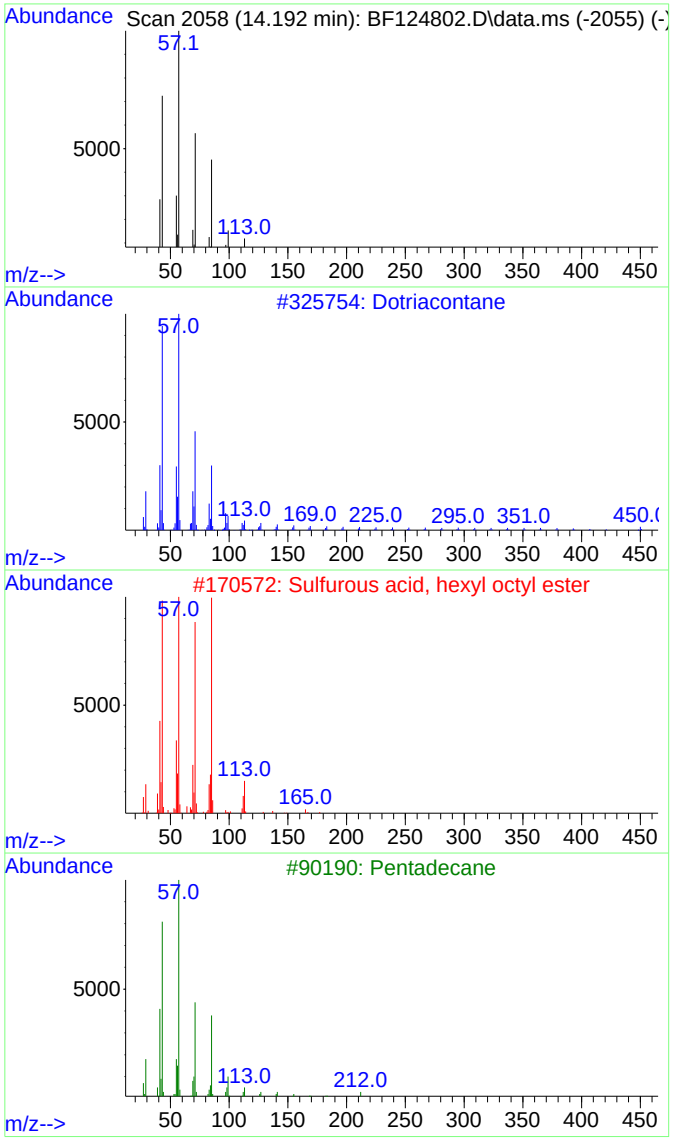
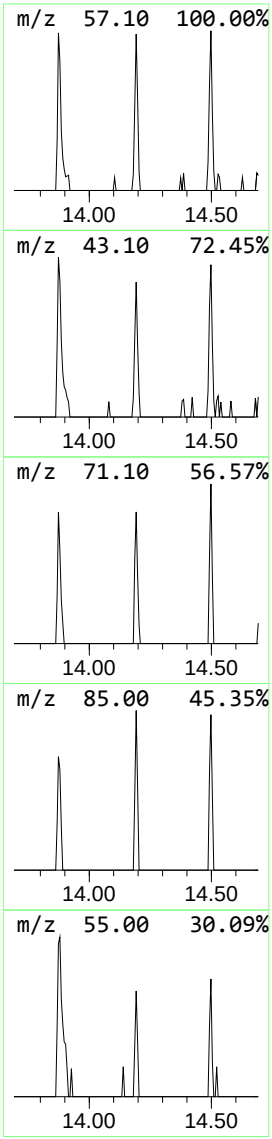
****

Peak Number 5 Dotriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	5.25 ng	12684	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dotriacontane	451	C32H66	000544-85-4	72
2	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64
3	Pentadecane	212	C15H32	000629-62-9	64
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	64
5	Tetradecane	198	C14H30	000629-59-4	64





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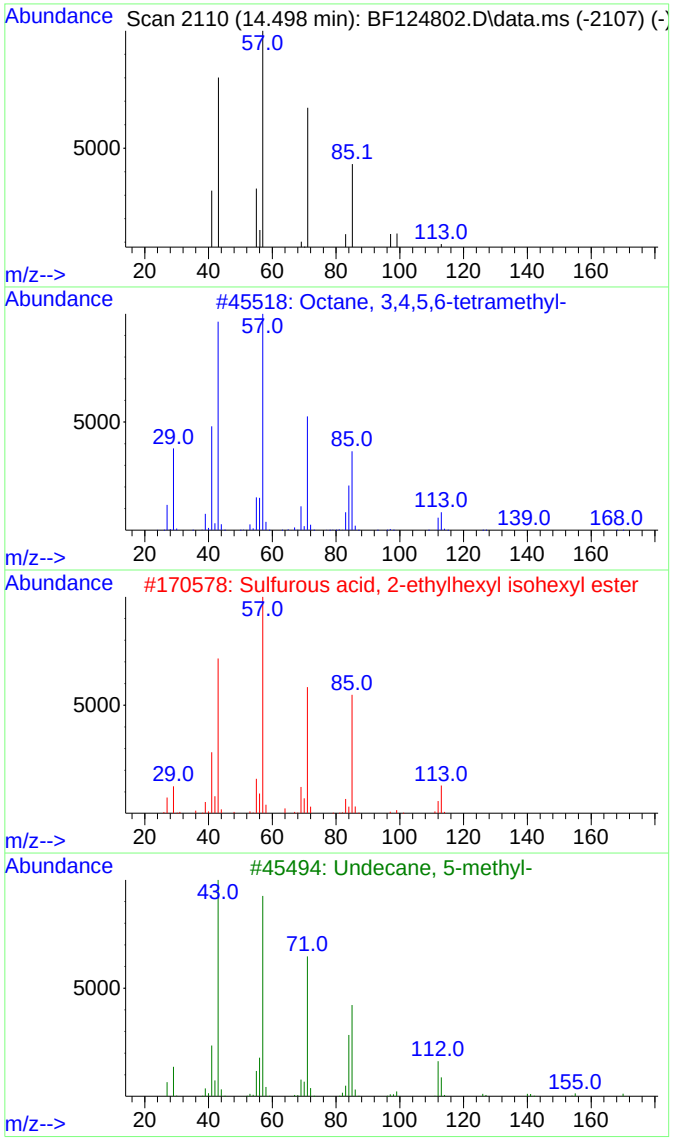
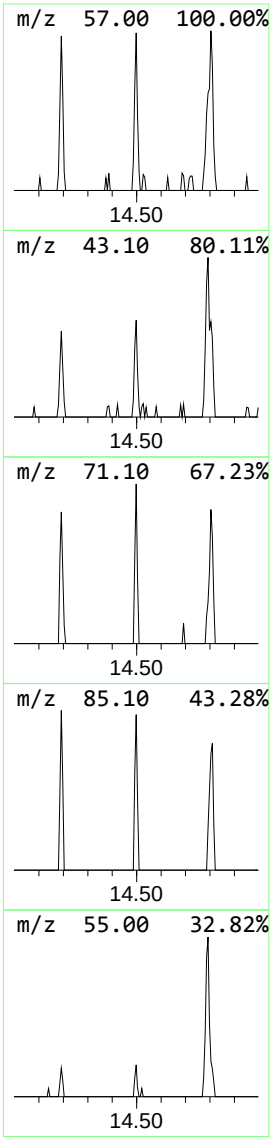
****

Peak Number 6 Octane, 3,4,5,6-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	5.35 ng	12925	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	72
2	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64
3	Undecane, 5-methyl-	170	C12H26	001632-70-8	59
4	Tetradecane	198	C14H30	000629-59-4	59
5	Hexadecane	226	C16H34	000544-76-3	59





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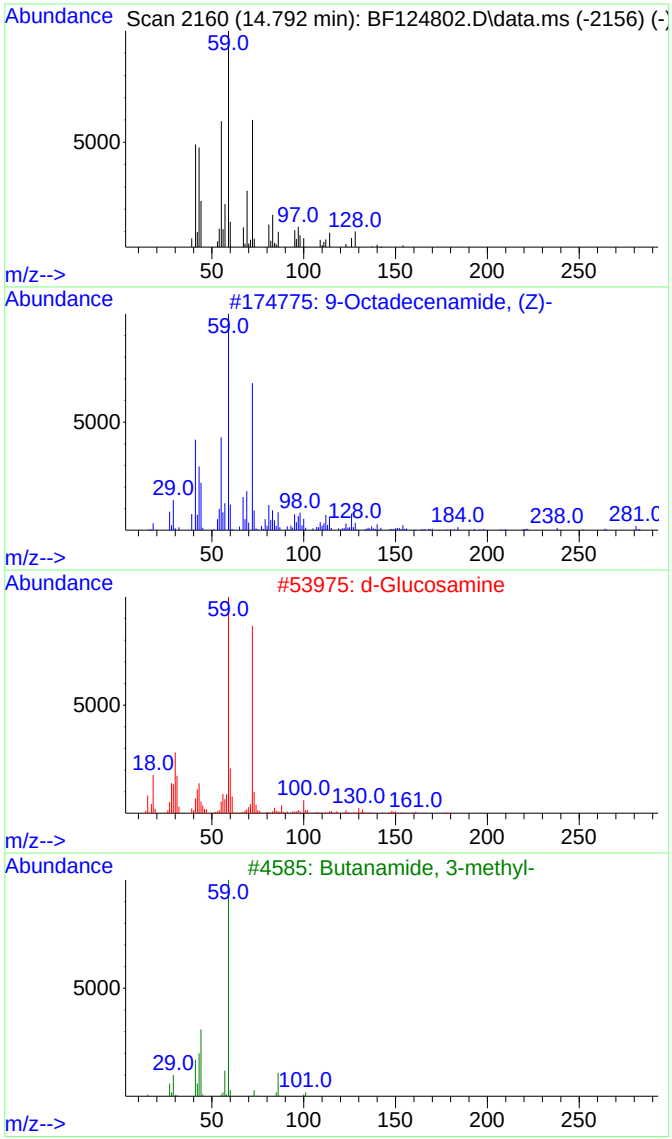
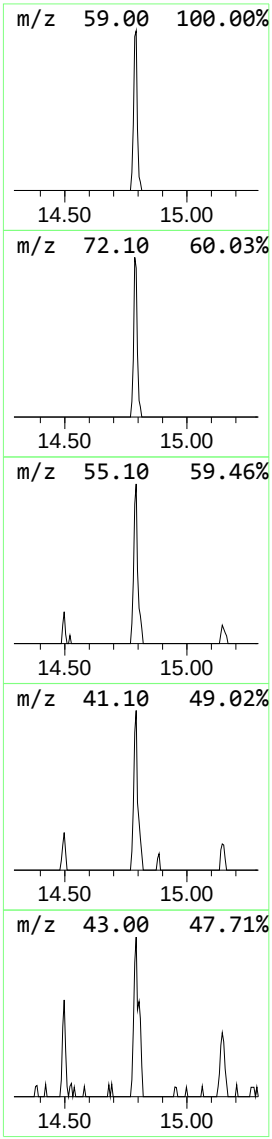
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	37.70 ng	84747	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2	d-Glucosamine	179	C6H13NO5	000090-77-7	47
3	Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	43
4	Pentanal, oxime	101	C5H11NO	000628-79-5	35
5	2-Pentanol, 3-chloro-2-methyl-	136	C6H13ClO	074685-49-7	35





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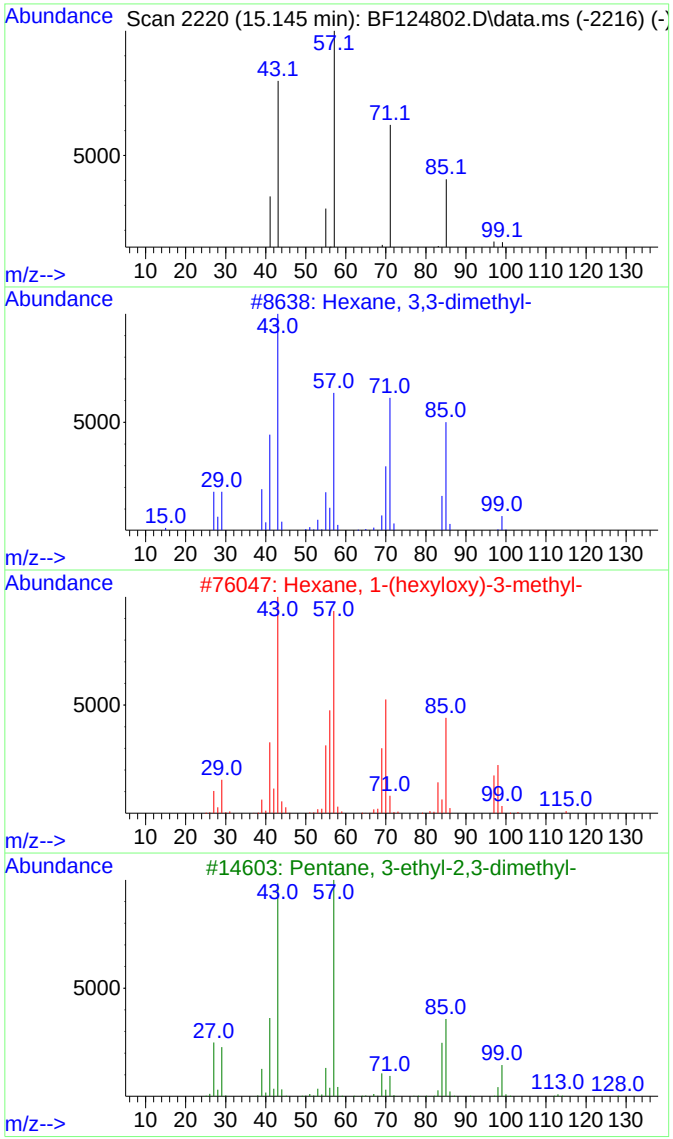
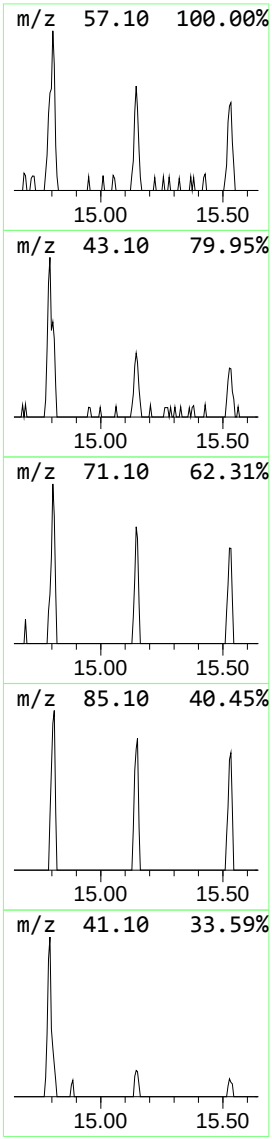
****

Peak Number 8 Hexane, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	5.54 ng	12451	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
2	Hexane, 1-(hexyloxy)-3-methyl-	200	C13H28O	074421-18-4	47
3	Pentane, 3-ethyl-2,3-dimethyl-	128	C9H20	016747-33-4	40
4	Ether, heptyl hexyl	200	C13H28O	007289-40-9	40
5	Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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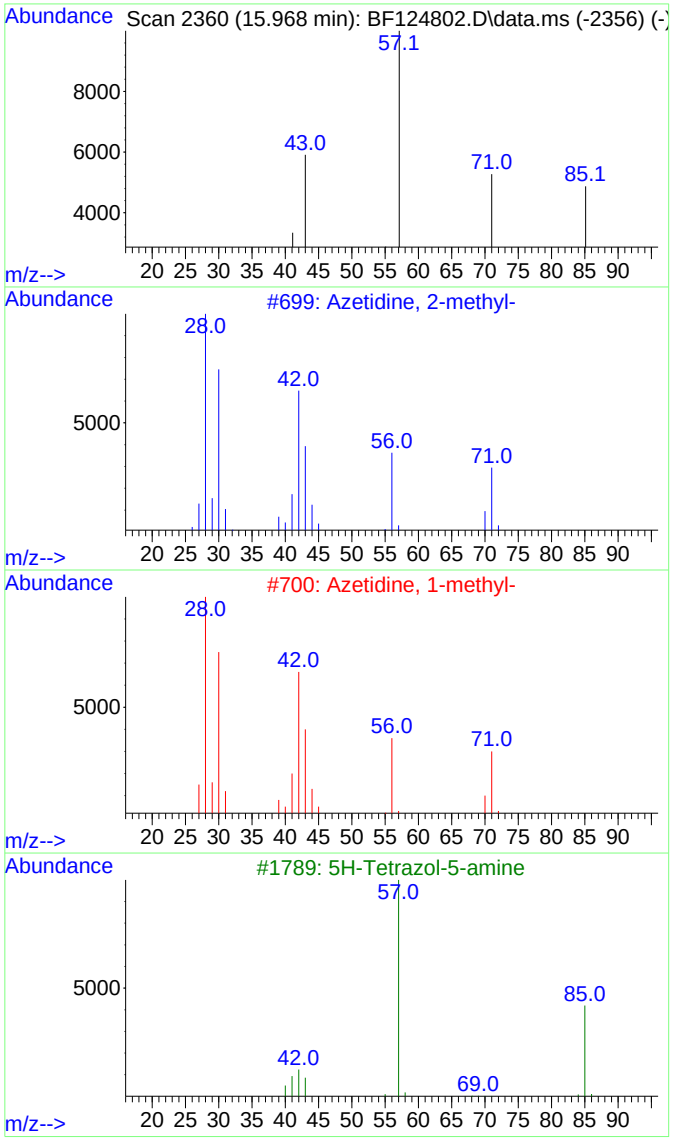
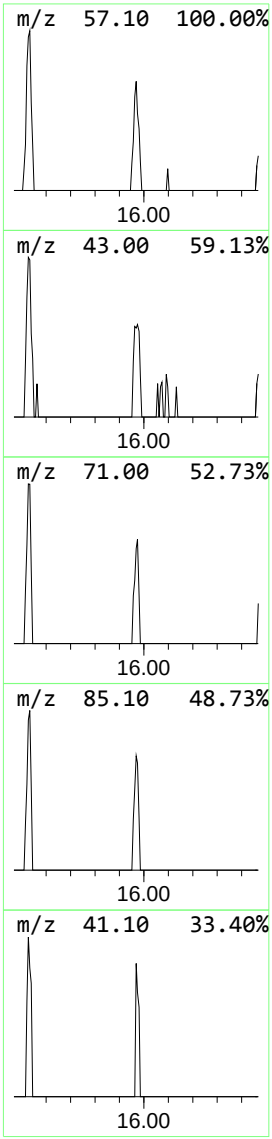
****

Peak Number 9 unknown15.968 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.968	2.93 ng	6596	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
2	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
3	5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	4
4	Cyclobutanone, oxime	85	C4H7NO	002972-05-6	4
5	2-Propenamide	71	C3H5NO	000079-06-1	4





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.128	9.0	ng	12142	1	6.869	26916	20.0
Ethanol, 2-(2-b...	8.051	9.5	ng	18115	2	8.151	38171	20.0
unknown11.916	11.916	2.2	ng	5927	4	11.398	54817	20.0
Carbonic acid, ...	13.874	10.7	ng	25923	5	14.033	48318	20.0
Dotriacontane	14.192	5.3	ng	12684	5	14.033	48318	20.0
Octane, 3,4,5,6...	14.498	5.3	ng	12925	5	14.033	48318	20.0
9-Octadecenamid...	14.792	37.7	ng	84747	6	15.509	44953	20.0
Hexane, 3,3-dim...	15.145	5.5	ng	12451	6	15.509	44953	20.0
unknown15.968	15.968	2.9	ng	6596	6	15.509	44953	20.0