LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128000.D
Acq On : 29 Apr 2022 17:44
Operator : CG\JU
Sample : N2609-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128000.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.551	549	555	558	rBV	2687059	2902245	80.19%	11.330%
2	6.551	719	725	728	rBV	2626296	3035577	83.87%	11.851%
3	6.922	784	788	791	rBV	894271	704341	19.46%	2.750%
4	7.486	878	884	887	rBV	2118818	2064311	57.03%	8.059%
5	8.204	1002	1006	1009	rBV	1091263	911344	25.18%	3.558%
6	9.280	1184	1189	1193	rBV	3615152	3619419	100.00%	14.130%
7	9.963	1300	1305	1309	rBV	1244035	1048423	28.97%	4.093%
8	10.757	1435	1440	1443	rBV	2465938	2200036	60.78%	8.589%
9	11.457	1555	1559	1561	rBV	1195530	1010769	27.93%	3.946%
10	11.480	1561	1563	1566	rVV	404713	299143	8.26%	1.168%
11	11.527	1566	1571	1575	rVB	51445	49873	1.38%	0.195%
12	11.686	1590	1598	1601	rBV2	34314	54384	1.50%	0.212%
13	11.968	1641	1646	1652	rBV3	163816	239756	6.62%	0.936%
14	12.068	1660	1663	1665	rBV2	76098	80271	2.22%	0.313%
15	12.504	1734	1737	1740	rBV	40934	44217	1.22%	0.173%
16	12.545	1740	1744	1749	rVV6	27856	52342	1.45%	0.204%
17	12.592	1749	1752	1757	rVV2	36014	38695	1.07%	0.151%
18	12.668	1762	1765	1769	rBV	525890	440686	12.18%	1.720%
19	12.898	1798	1804	1808	rBV	404891	448769	12.40%	1.752%
20	12.951	1808	1813	1822	rVV	99713	229687	6.35%	0.897%
21	13.045	1824	1829	1832	rVV	3276631	2903769	80.23%	11.336%
22	13.115	1837	1841	1845	rVB2	31850	47379	1.31%	0.185%
23	13.227	1857	1860	1863	rVB	53386	52658	1.45%	0.206%
24	13.333	1874	1878	1880	rBV2	50115	48198	1.33%	0.188%
25	13.474	1896	1902	1906	rBV2	74173	129171	3.57%	0.504%
26	13.515	1906	1909	1915	rVB	82804	96988	2.68%	0.379%
27	13.733	1943	1946	1951	rVB	36061	41229	1.14%	0.161%
28	13.851	1961	1966	1968	rBV3	40524	51629	1.43%	0.202%
29	13.945	1978	1982	1985	rVB2	30383	40591	1.12%	0.158%
30	14.021	1990	1995	1996	rBV2	41093	56580	1.56%	0.221%
31	14.098	2004	2008	2011	rBV2	694001	775566	21.43%	3.028%
32	14.127	2011	2013	2020	rVB	173025	158330	4.37%	0.618%
33	14.204	2020	2026	2028	rBV3	30199	46510	1.29%	0.182%
34	14.486	2071	2074	2078	rBV3	42298	43413	1.20%	0.169%
35	15.157	2184	2188	2192	rBV	151637	249269	6.89%	0.973%
36	15.221	2196	2199	2204	rVB3	45143	60395	1.67%	0.236%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
WC-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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.474	2239	2242	2249	rVB	98547	131030	3.62%	0.512%
38	15.539	2249	2253	2259	rBV	130030	158914	4.39%	0.620%
39	15.609	2259	2265	2278	rVB	509424	728391	20.12%	2.844%
40	16.074	2341	2344	2349	rVB	38415	52028	1.44%	0.203%
41	17.133	2519	2524	2532	rVB2	56641	117343	3.24%	0.458%
42	17.227	2537	2540	2547	rVB4	30943	55493	1.53%	0.217%
43	17.598	2599	2603	2611	rVB	44115	95467	2.64%	0.373%

Sum of corrected areas: 25614629

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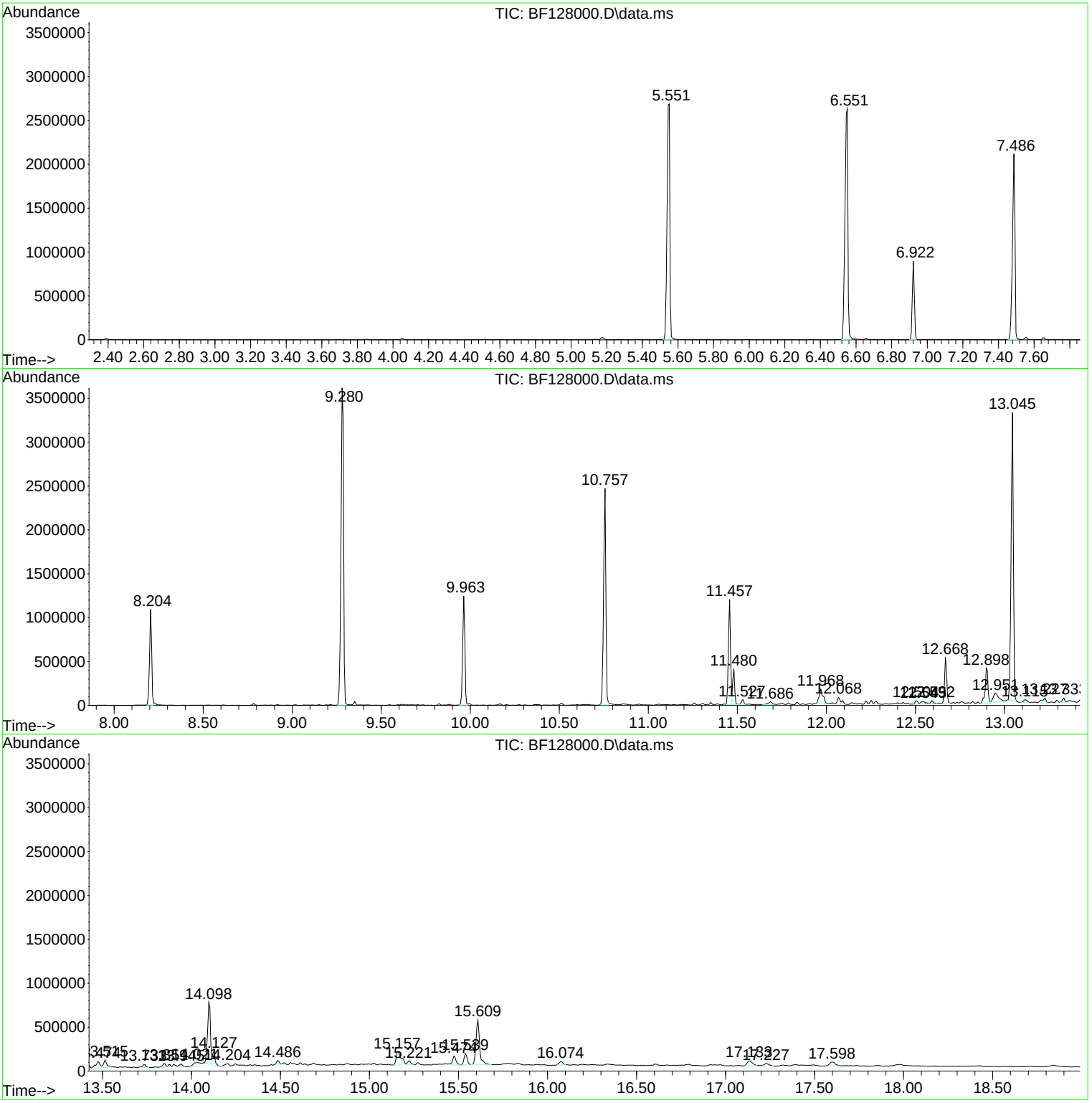
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128000.D
Acq On : 29 Apr 2022 17:44
Operator : CG\JU
Sample : N2609-04
Misc :
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Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

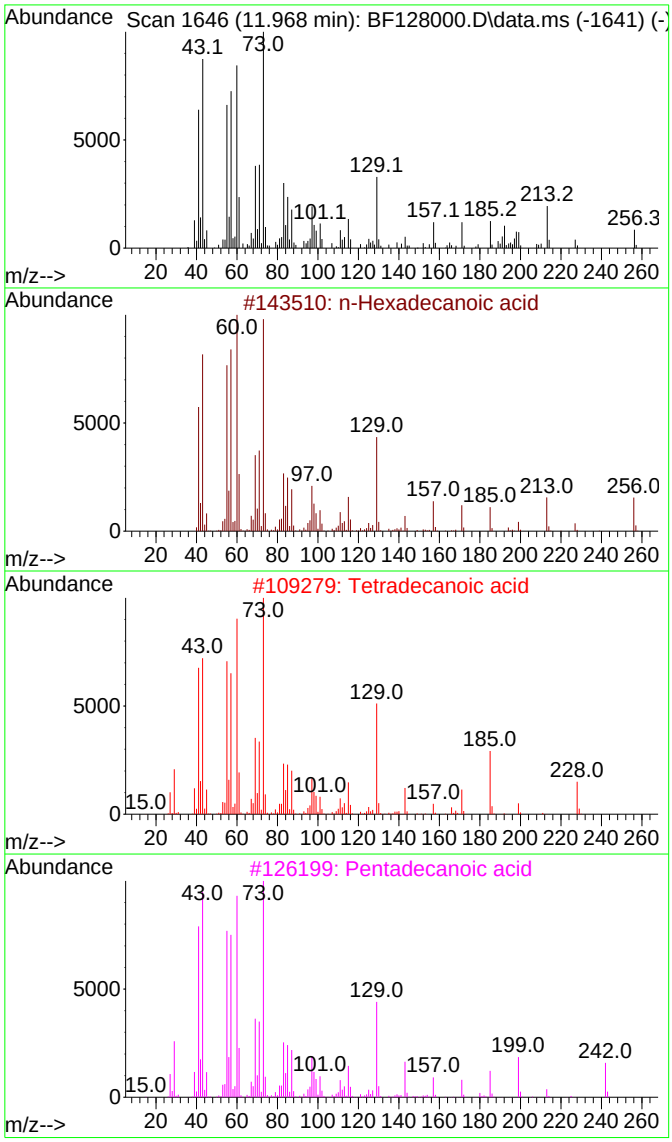
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

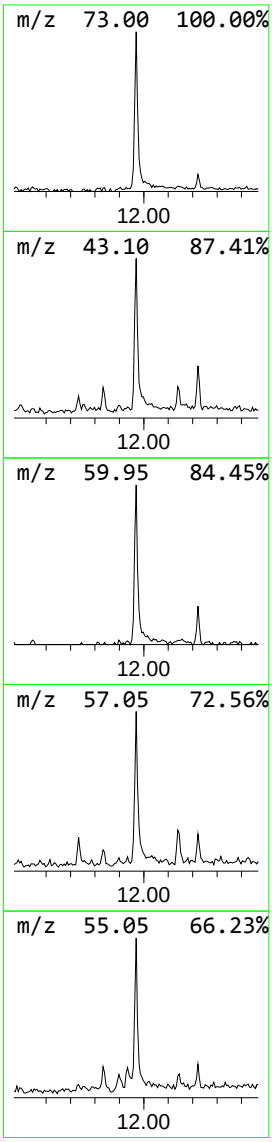
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	4.74 ng	239756	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
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Acq On : 29 Apr 2022 17:44
Operator : CG\JU
Sample : N2609-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
WC-2

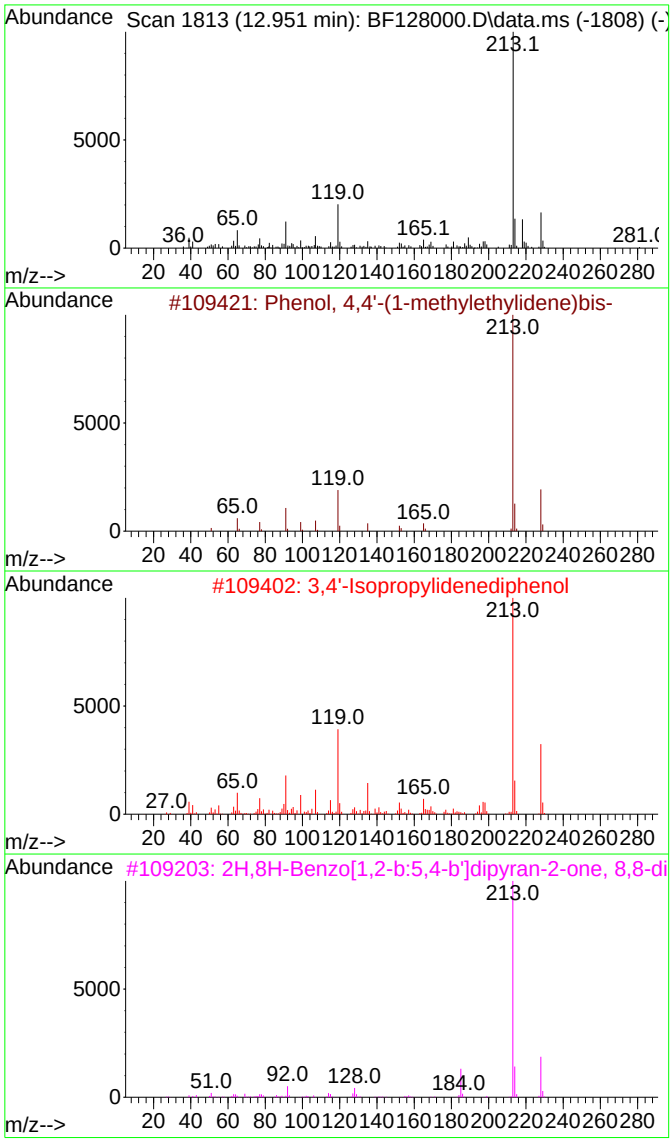
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

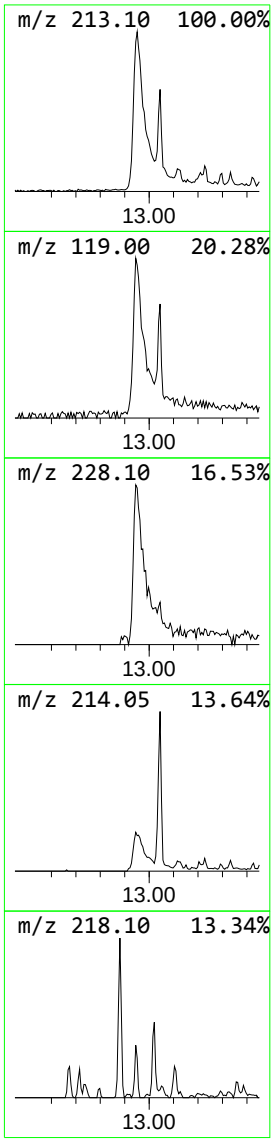
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Phenol, 4,4'-(1-methylethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.951	5.92 ng	229687	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	78
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	58
4	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	53
5	Isonicotinic acid, phenylmethyl ...	213	C13H11NO2	1000308-34-6	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF128000.D
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Sample : N2609-04
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Instrument :
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ClientSampleId :
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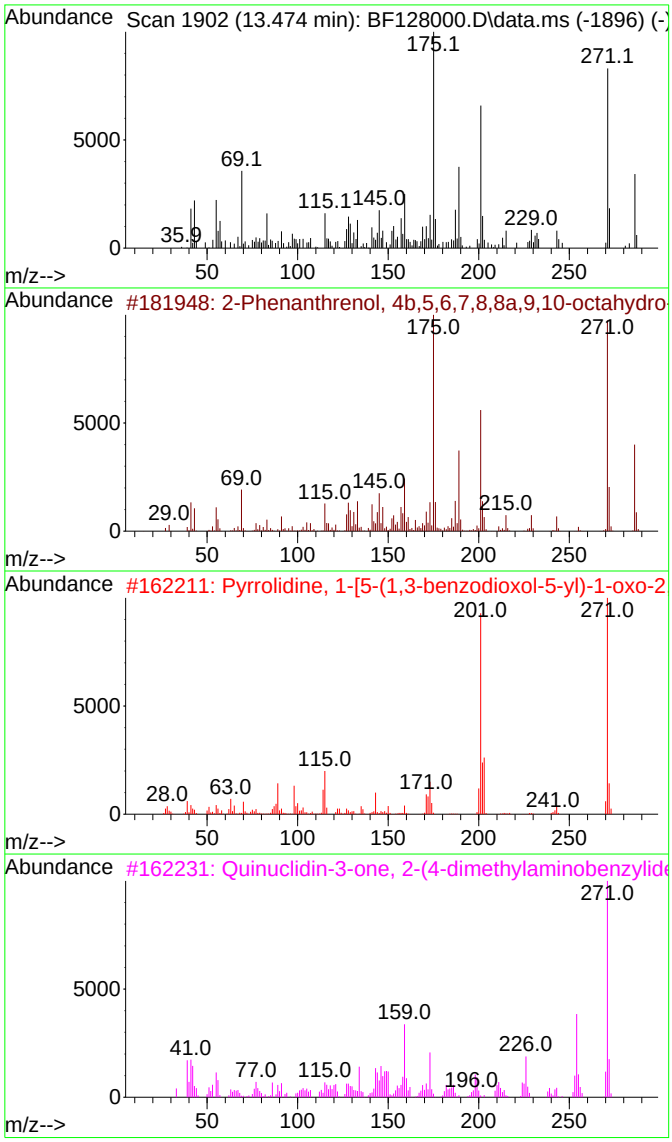
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

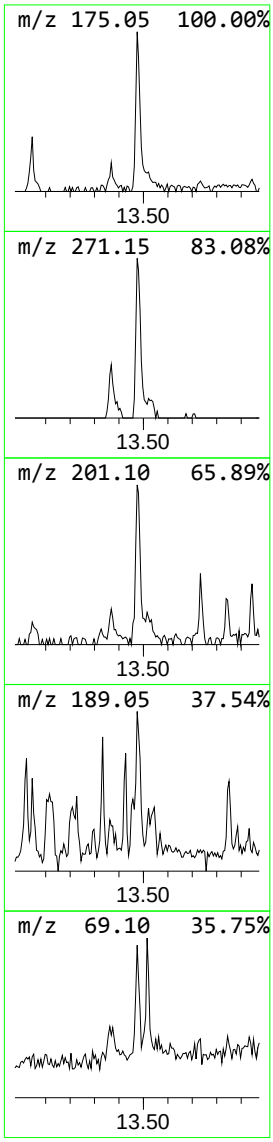
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.474	3.33 ng	129171	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	35
3	Quinuclidin-3-one, 2-(4-dimethyl...	271	C16H21N3O	1000266-14-6	25
4	Crinan-1-ol, 2,3-didehydro-,(1.a...	271	C16H17NO3	1000111-31-3	25
5	Crinan-1-one	271	C16H17NO3	098301-98-5	22





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Sample : N2609-04
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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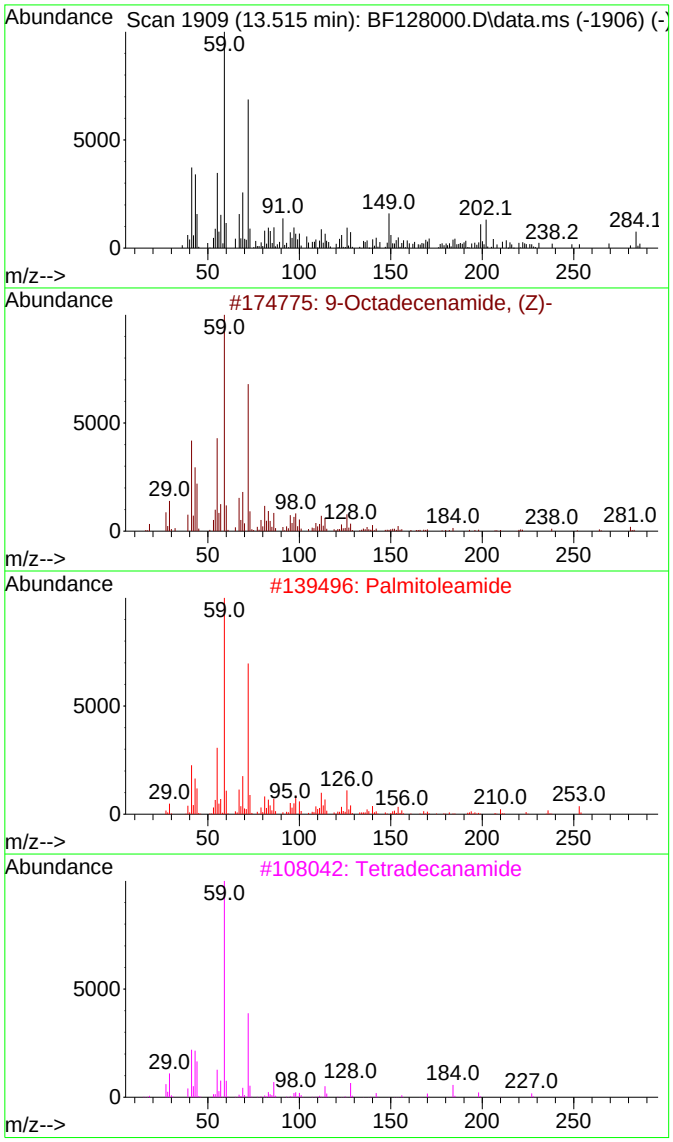
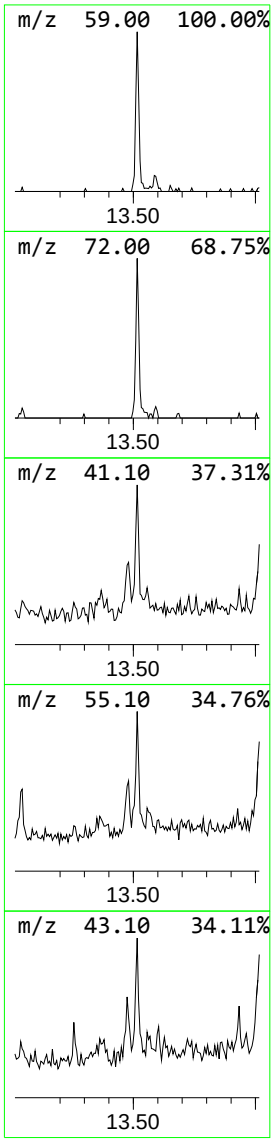
Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.515	2.50 ng	96988	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Palmitoleamide	253	C16H31NO	106010-22-4	58
3	Tetradecanamide	227	C14H29NO	000638-58-4	55
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	52
5	Silane, (chloromethyl)dimethyl-	108	C3H9ClSi	003144-74-9	35





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Sample : N2609-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

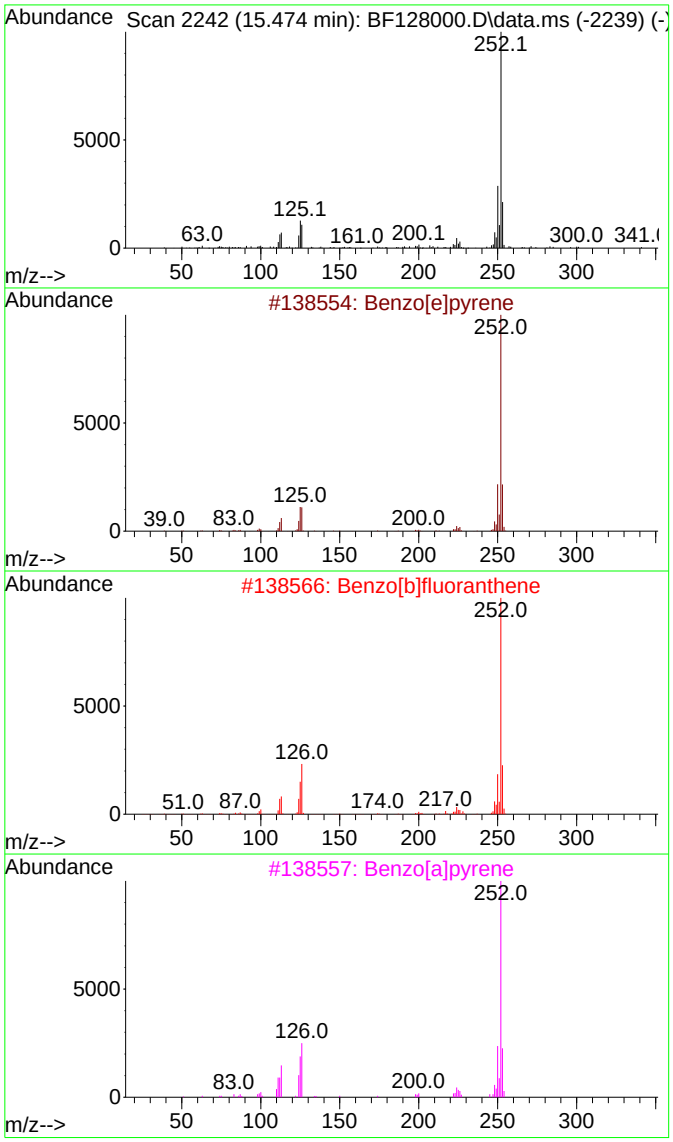
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

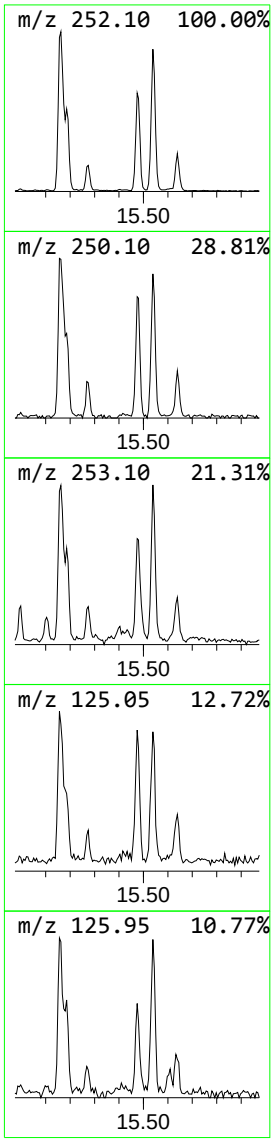
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.474	3.60 ng	131030	Perylene-d12	15.609

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	90
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





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
n-Hexadecanoic ...	11.969	4.7	ng	239756	4	11.457	1010770	20.0
Phenol, 4,4'-(1...	12.951	5.9	ng	229687	5	14.098	775566	20.0
2-Phenanthrenol...	13.474	3.3	ng	129171	5	14.098	775566	20.0
9-Octadecenamid...	13.515	2.5	ng	96988	5	14.098	775566	20.0
Benzo[e]pyrene	15.474	3.6	ng	131030	6	15.609	728391	20.0